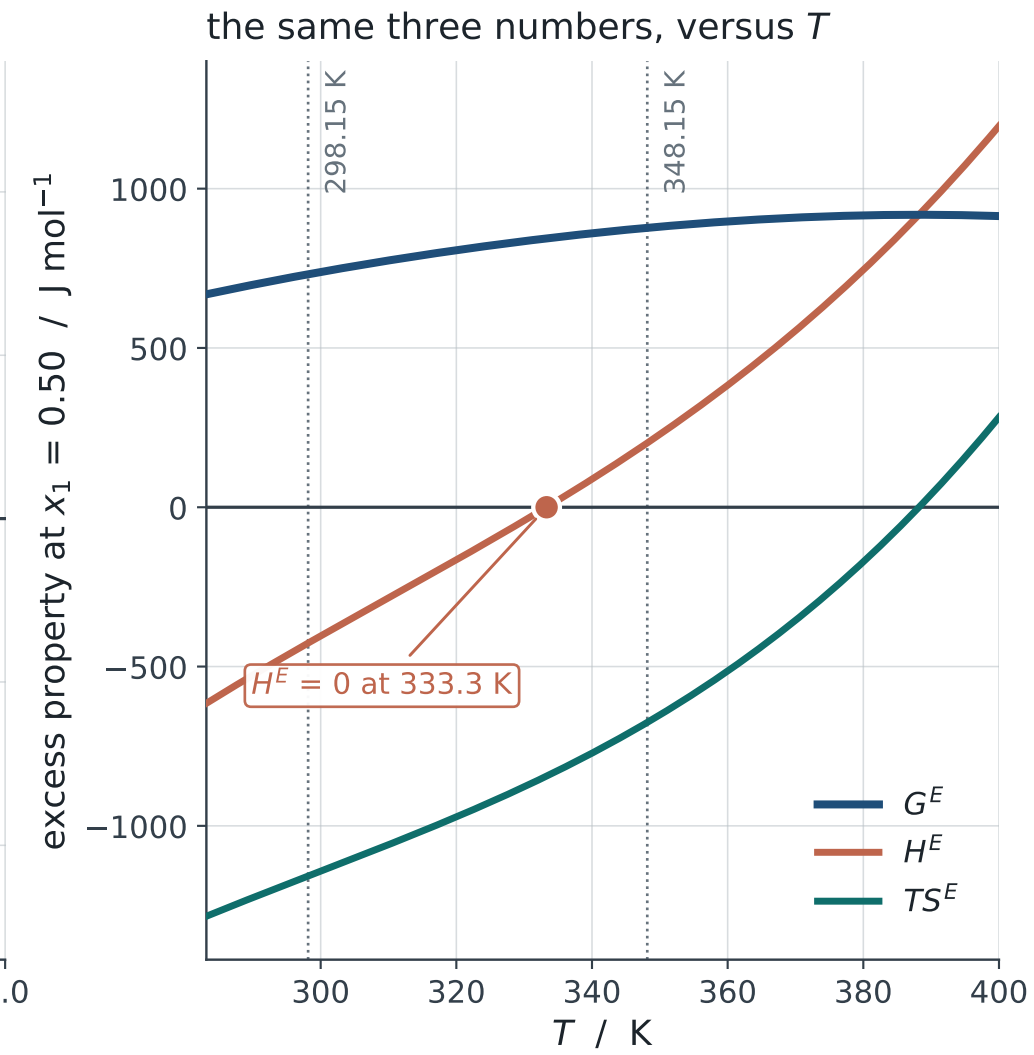
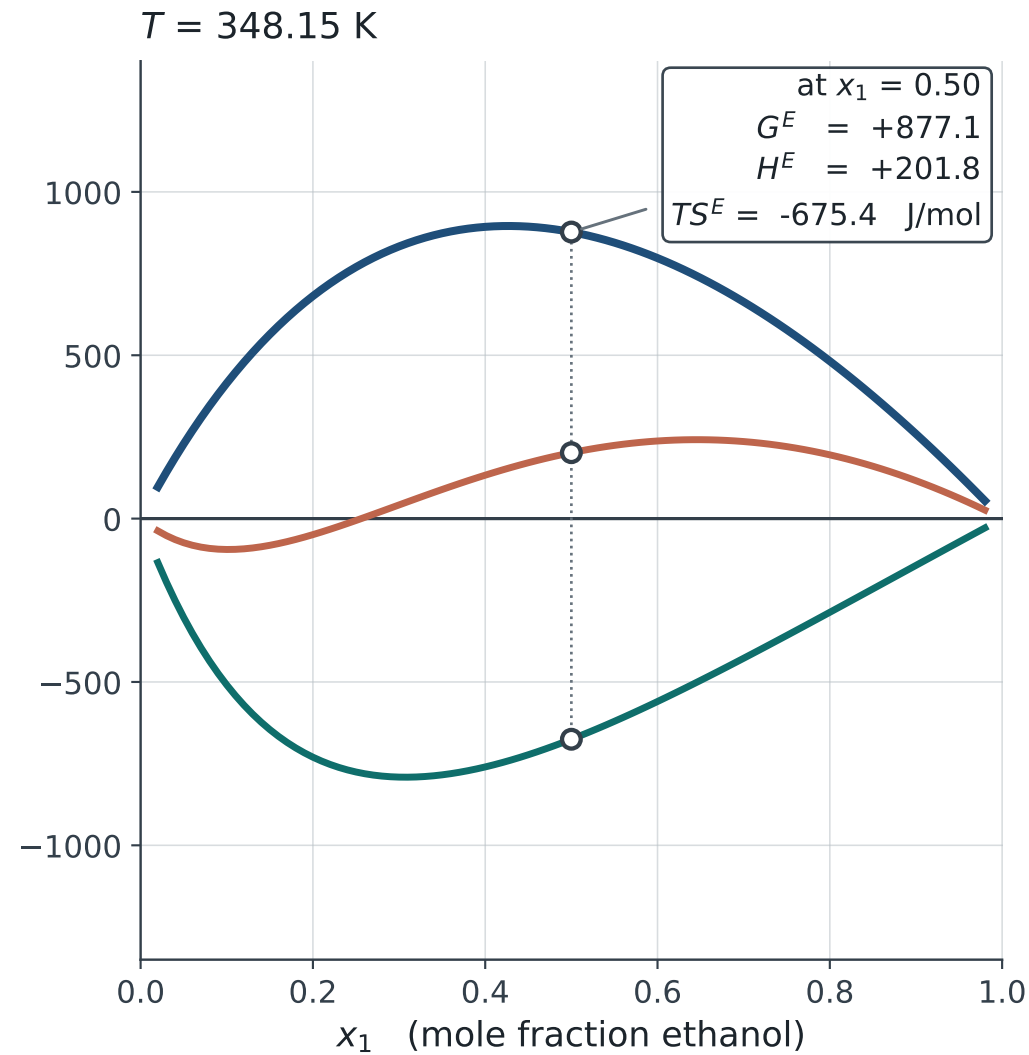
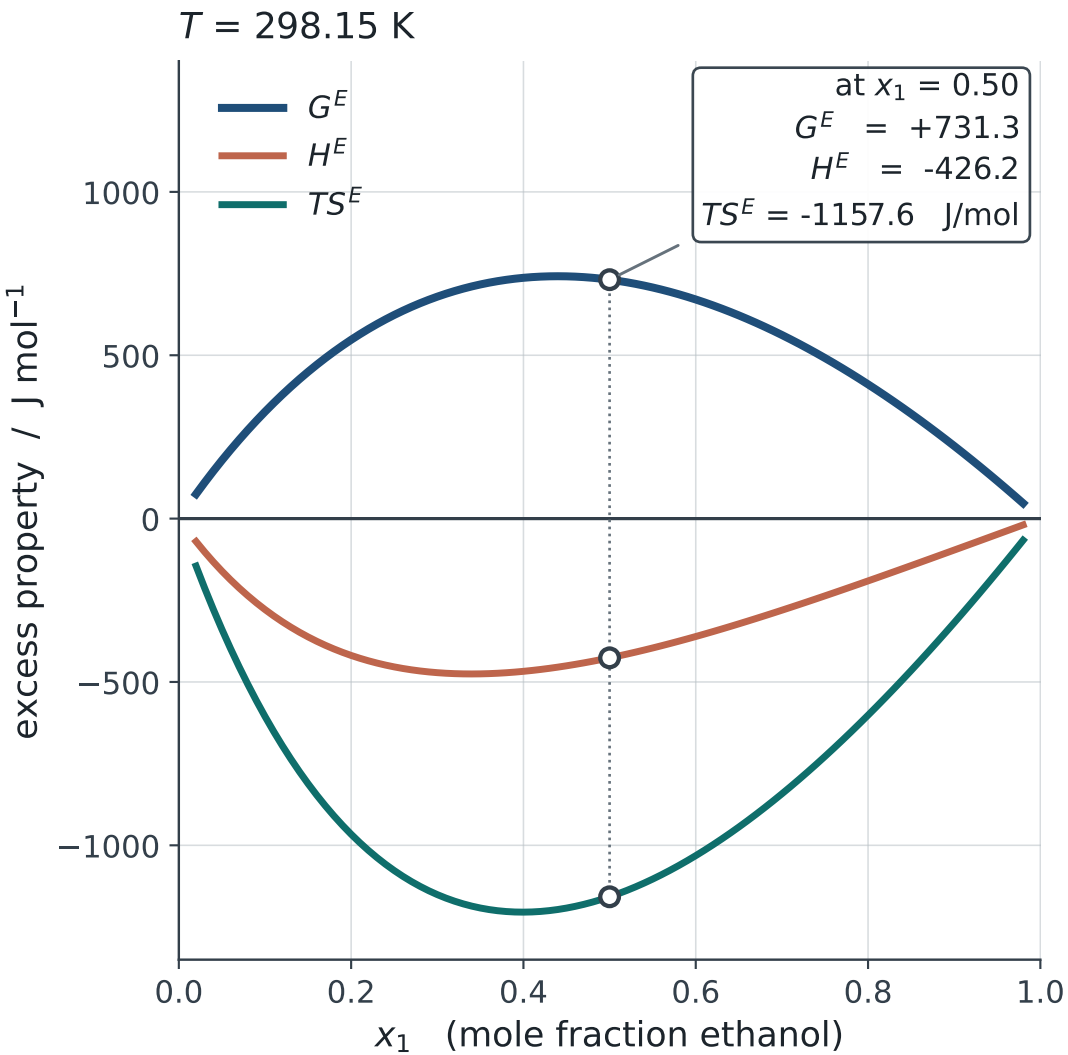


G^E is positive because of entropy, not energy — and which term dominates is a function of temperature

ethanol (1) + water (2), modified UNIFAC (Dortmund)

At 298.15 K mixing gives out heat ($H^E = -426$ J/mol at $x_1 = 0.5$) and every joule of the positive G^E , and more, comes from $-TS^E$. By 348.15 K H^E has changed sign: G^E moved only +146 J/mol while its two parts moved +628 and +482.



H^E IS NOT MEASURED HERE. It is obtained from the temperature dependence of the model, $H^E = -RT^2 \partial(G^E/RT)/\partial T$. The model is modified UNIFAC (Dortmund) —

`thermo.unifac.UNIFAC`, DOUFIP2006 table, DOUFSG subgroups — whose temperature-dependent group parameters were regressed simultaneously against VLE, LLE, h^E and γ^∞ data (Gmehling, Li & Schiller, *Ind. Eng. Chem. Res.* 1993, 32(1), doi:10.1021/ie00013a024), which is why its temperature derivative is worth plotting at all. `thermo`'s analytic HE() was checked against a central difference of GE() alone over 97 compositions at both temperatures: largest disagreement 3.94e-06 J/mol. No parameter here is fitted or assumed; ethanol and water enter as UNIFAC subgroups only.