2-(N-Ethyl-N-tolylamino)ethanol, pentafluoropropionate

Inchi: InChI=1S/C14H16F5NO2/c1-3-20(11-6-4-5-10(2)9-11)7-8-22-12(21)13(15,16)14(17,18)1

InchiKey: YPTCRXCWUSFWBX-UHFFFAOYSA-N

Formula: C14H16F5NO2

SMILES: CCN(CCOC(=O)C(F)(F)C(F)(F)F)c1cccc(C)c1

Mol. weight [g/mol]: 325.27

Physical Properties

Property code	Value	Unit	Source
gf	-921.73	kJ/mol	Joback Method
hf	-1282.55	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.562		Crippen Method
mcvol	210.630	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1484.00		NIST Webbook
tb	630.00	K	Joback Method
tc	809.20	K	Joback Method
tf	398.90	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.25	J/mol×K	630.00	Joback Method
cpg	592.66	J/mol×K	659.87	Joback Method
cpg	606.16	J/mol×K	689.73	Joback Method
cpg	618.78	J/mol×K	719.60	Joback Method
cpg	630.59	J/mol×K	749.47	Joback Method
cpg	641.62	J/mol×K	779.33	Joback Method
cpg	651.93	J/mol×K	809.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume