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

Inchi: InChI=1S/C15H16F7NO2/c1-3-23(11-6-4-5-10(2)9-11)7-8-25-12(24)13(16,17)14(18,19)1

InchiKey: PTGIOONROYONRR-UHFFFAOYSA-N

Formula: C15H16F7NO2

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

Mol. weight [g/mol]: 375.28

Physical Properties

Property code	Value	Unit	Source
gf	-1300.09	kJ/mol	Joback Method
hf	-1704.16	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.197		Crippen Method
mcvol	228.260	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	648.19	K	Joback Method
tc	821.52	K	Joback Method
tf	413.77	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.41	J/mol×K	648.19	Joback Method
cpg	663.58	J/mol×K	677.08	Joback Method
cpg	676.80	J/mol×K	705.97	Joback Method
cpg	689.14	J/mol×K	734.85	Joback Method
cpg	700.66	J/mol×K	763.74	Joback Method
cpg	711.40	J/mol×K	792.63	Joback Method
cpg	721.43	J/mol×K	821.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374921&Units=SI

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