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

Inchi: InChI=1S/C13H16F3NO2/c1-3-17(11-6-4-5-10(2)9-11)7-8-19-12(18)13(14,15)16/h4-6,9H

InchiKey: VOTYPCCKAXDIQK-UHFFFAOYSA-N

Formula: C13H16F3NO2

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

Mol. weight [g/mol]: 275.27

Physical Properties

Property code	Value	Unit	Source
gf	-543.37	kJ/mol	Joback Method
hf	-860.94	kJ/mol	Joback Method
hfus	30.71	kJ/mol	Joback Method
hvap	54.92	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.927		Crippen Method
mcvol	193.000	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
tb	611.81	K	Joback Method
tc	798.28	K	Joback Method
tf	384.03	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.87	J/mol×K	611.81	Joback Method
cpg	522.47	J/mol×K	642.89	Joback Method
cpg	536.19	J/mol×K	673.97	Joback Method
cpg	549.07	J/mol×K	705.05	Joback Method
cpg	561.16	J/mol×K	736.13	Joback Method
cpg	572.47	J/mol×K	767.21	Joback Method
cpg	583.06	J/mol×K	798.28	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=U374919&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