1-Aminotetradecane, N-trifluoroacetyl

Other names: 1-Aminotetradecane, TFA
Inchi: InChI=1S/C16H30F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-15(21)16(17,18)19/h2-14
InchiKey: MQMIATHAPLUUAU-UHFFFAOYSA-N
Formula: C16H30F3NO
SMILES: CCCCCCCCCCCCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 309.41
CAS: 1995-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-537.28	kJ/mol	Joback Method
hf	-1029.76	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	60.64	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.366		Crippen Method
mcvol	253.160	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	664.10	K	Joback Method
tc	826.47	K	Joback Method
tf	376.86	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.19	J/mol×K	664.10	Joback Method
cpg	750.88	J/mol×K	691.16	Joback Method
cpg	766.79	J/mol×K	718.22	Joback Method
cpg	781.94	J/mol×K	745.29	Joback Method
cpg	796.36	J/mol×K	772.35	Joback Method

cpg	810.09	J/mol×K	799.41	Joback Method
cpg	823.16	J/mol×K	826.47	Joback Method

Sources

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=C1995024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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