

1-Aminoheptadecane, N-trifluoroacetyl-

Other names:	1-Aminoheptadecane, TFA
Inchi:	InChI=1S/C19H36F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-18(24)19(20,21)
InchiKey:	RGNMEQXMHOFJSX-UHFFFAOYSA-N
Formula:	C19H36F3NO
SMILES:	CCCCCCCCCCCCCCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]:	351.49

Physical Properties

Property code	Value	Unit	Source
gf	-512.02	kJ/mol	Joback Method
hf	-1091.68	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.536		Crippen Method
mcvol	295.430	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2139.00		NIST Webbook
tb	732.74	K	Joback Method
tc	900.85	K	Joback Method
tf	410.67	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.53	J/molxK	732.74	Joback Method
cpg	925.63	J/molxK	760.76	Joback Method
cpg	942.83	J/molxK	788.78	Joback Method
cpg	959.19	J/molxK	816.80	Joback Method
cpg	974.75	J/molxK	844.82	Joback Method
cpg	989.54	J/molxK	872.83	Joback Method
cpg	1003.60	J/molxK	900.85	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=U360368&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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