N-Hexadecyltrifluoroacetamide

Other names: 1-Aminohexadecane, TFA
Inchi: InChI=1S/C18H34F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-17(23)18(19,20)21
InchiKey: BSBDOZVBTYWNPH-UHFFFAOYSA-N
Formula: C18H34F3NO
SMILES: CCCCCCCCCCCCCCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 337.46
CAS: 1994-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-520.44	kJ/mol	Joback Method
hf	-1071.04	kJ/mol	Joback Method
hfus	50.90	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.146		Crippen Method
mcvol	281.340	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	709.86	K	Joback Method
tc	875.49	K	Joback Method
tf	399.40	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.70	J/mol×K	709.86	Joback Method
cpg	866.31	J/mol×K	737.46	Joback Method
cpg	883.07	J/mol×K	765.07	Joback Method
cpg	899.02	J/mol×K	792.67	Joback Method
cpg	914.19	J/mol×K	820.28	Joback Method
cpg	928.62	J/mol×K	847.88	Joback Method

cpg	942.35	J/mol×K	875.49	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=C1994485&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