1-Aminooctadecane, TFA

Inchi: InChI=1S/C20H38F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-24-19(25)20(21
InchiKey: ZTMLPTAIGWNQQB-UHFFFAOYSA-N
Formula: C20H38F3NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 365.52

Physical Properties

Property code	Value	Unit	Source
gf	-503.60	kJ/mol	Joback Method
hf	-1112.32	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.926		Crippen Method
mcvol	309.520	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	755.62	K	Joback Method
tc	926.87	K	Joback Method
tf	421.94	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.32	J/mol×K	755.62	Joback Method
cpg	985.93	J/mol×K	784.16	Joback Method
cpg	1003.61	J/mol×K	812.70	Joback Method
cpg	1020.41	J/mol×K	841.25	Joback Method
cpg	1036.36	J/mol×K	869.79	Joback Method
cpg	1051.52	J/mol×K	898.33	Joback Method
cpg	1065.93	J/mol×K	926.87	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=R571083&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