1-Aminopentadecane, TFA

Inchi: InChI=1S/C17H32F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-16(22)17(18,19)20/h2
InchiKey: YWUGCTYVGKBRBI-UHFFFAOYSA-N
Formula: C17H32F3NO
SMILES: CCCCCCCCCCCCCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 323.44

Physical Properties

Property code	Value	Unit	Source
gf	-528.86	kJ/mol	Joback Method
hf	-1050.40	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.756		Crippen Method
mcvol	267.250	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	1941.00		NIST Webbook
tb	686.98	K	Joback Method
tc	850.71	K	Joback Method
tf	388.13	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.89	J/mol×K	686.98	Joback Method
cpg	808.04	J/mol×K	714.27	Joback Method
cpg	824.37	J/mol×K	741.56	Joback Method
cpg	839.92	J/mol×K	768.85	Joback Method
cpg	854.71	J/mol×K	796.14	Joback Method
cpg	868.79	J/mol×K	823.43	Joback Method
cpg	882.19	J/mol×K	850.71	Joback Method

Sources

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=R571098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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