6-Methyl-6-heptadecaneamine TFA

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

Physical Properties

Property code	Value	Unit	Source
gf	-500.76	kJ/mol	Joback Method
hf	-1121.07	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.925		Crippen Method
mcvol	309.520	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	1981.00		NIST Webbook
rinpol	1981.00		NIST Webbook
tb	752.39	K	Joback Method
tc	925.41	K	Joback Method
tf	424.36	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.73	J/mol×K	752.39	Joback Method
cpg	987.33	J/mol×K	781.23	Joback Method
cpg	1004.96	J/mol×K	810.06	Joback Method
cpg	1021.69	J/mol×K	838.90	Joback Method
cpg	1037.58	J/mol×K	867.74	Joback Method
cpg	1052.68	J/mol×K	896.57	Joback Method
cpg	1067.05	J/mol×K	925.41	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=R571147&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