Perfluoromethyldiethylamine

Inchi: InChI=1S/C5F13N/c6-1(7,8)3(12,13)19(5(16,17)18)4(14,15)2(9,10)11
InchiKey: KMPITNDOTGKQSE-UHFFFAOYSA-N
Formula: C5F13N
SMILES: FC(F)(F)N(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 321.04
CAS: 758-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-2416.33	kJ/mol	Joback Method
hf	-2672.18	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	29.40 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.59		Crippen Method
logp	4.118		Crippen Method
mcvol	114.300	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
sl	475.09	J/mol×K	NIST Webbook
tb	300.60	K	Joback Method
tc	409.55	K	Joback Method
tf	150.10 ± 0.20	K	NIST Webbook
tt	149.64 ± 0.02	K	NIST Webbook
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.41	J/mol×K	300.60	Joback Method
cpg	257.16	J/mol×K	318.76	Joback Method
cpg	268.28	J/mol×K	336.92	Joback Method
cpg	278.80	J/mol×K	355.07	Joback Method
cpg	288.75	J/mol×K	373.23	Joback Method
cpg	298.13	J/mol×K	391.39	Joback Method
cpg	306.96	J/mol×K	409.55	Joback Method

cpl	337.46	J/mol×K	298.15	NIST Webbook
hfust	4.60	kJ/mol	150.10	NIST Webbook
hfust	7.16	kJ/mol	149.70	NIST Webbook
sfust	30.60	J/mol×K	150.10	NIST Webbook

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=C758485&Units=SI

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust: Entropy of fusion at a given temperature
sl: Liquid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume