PERFLUORO-3-METHYLPENTANE

Inchi: InChI=1S/C6HF13/c7-2(8,5(14,15)16)1(4(11,12)13)3(9,10)6(17,18)19/h1H
InchiKey: DGSHCVBIHBUFNY-UHFFFAOYSA-N
Formula: C6HF13
SMILES: FC(F)(F)C(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 320.05

Physical Properties

Property code	Value	Unit	Source
af	0.4760		KDB
gf	-2521.13	kJ/mol	Joback Method
hf	-2765.63	kJ/mol	Joback Method
hfus	10.74	kJ/mol	Joback Method
hvap	11.46	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.560		Crippen Method
mcvol	118.410	ml/mol	McGowan Method
pc	1690.00	kPa	KDB
tb	331.52	K	KDB
tc	450.00	K	KDB
tf	162.15	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.44	J/mol×K	310.60	Joback Method
cpg	269.31	J/mol×K	329.39	Joback Method
cpg	280.54	J/mol×K	348.18	Joback Method
cpg	291.16	J/mol×K	366.97	Joback Method
cpg	301.20	J/mol×K	385.76	Joback Method
cpg	310.66	J/mol×K	404.55	Joback Method
cpg	319.57	J/mol×K	423.34	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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1629.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume