Perfluorohexamethylprismane

Inchi: InChI=1S/C12F18/c13-7(14,15)1-2(8(16,17)18)3(1,9(19,20)21)6(12(28,29)30)4(1,10(22,2
InchiKey: JFELTPAOLMOQHL-UHFFFAOYSA-N
Formula: C12F18
SMILES: FC(F)(F)C12C3(C(F)(F)F)C1(C(F)(F)F)C1(C(F)(F)F)C2(C(F)(F)F)C31C(F)(F)F
Mol. weight [g/mol]: 486.10
CAS: 22736-20-5

Physical Properties

Property code	Value	Unit	Source
gf	-3172.14	kJ/mol	Joback Method
hf	-3494.57	kJ/mol	Joback Method
hfus	7.29	kJ/mol	Joback Method
hvap	10.92	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.333		Crippen Method
mcvol	168.360	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
tb	434.88	K	Joback Method
tc	565.08	K	Joback Method
tf	477.94	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.59	J/mol×K	521.68	Joback Method
cpg	572.20	J/mol×K	543.38	Joback Method
cpg	512.72	J/mol×K	434.88	Joback Method
cpg	528.26	J/mol×K	456.58	Joback Method
cpg	541.80	J/mol×K	478.28	Joback Method
cpg	553.51	J/mol×K	499.98	Joback Method
cpg	579.55	J/mol×K	565.08	Joback Method
hsubt	49.20	kJ/mol	299.50	NIST Webbook
hvapt	33.10	kJ/mol	333.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22736205&Units=SI
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

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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