Perfluorohxamethyl benzvalene

Inchi: InChI=1S/C12F18/c13-5(14,15)1-2(6(16,17)18)4(10(22,23)24)7(11(25,26)27)3(1,9(19,20
InchiKey: FICGHCVUNRMIDX-UHFFFAOYSA-N
Formula: C12F18
SMILES: FC(F)(F)C1=C(C(F)(F)F)C2(C(F)(F)F)C3(C(F)(F)F)C1(C(F)(F)F)C23C(F)(F)F
Mol. weight [g/mol]: 486.10
CAS: 22186-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-3239.80	kJ/mol	Joback Method
hf	-3561.15	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	15.75	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.643		Crippen Method
mcvol	174.920	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
tb	454.26	K	Joback Method
tc	583.91	K	Joback Method
tf	431.68	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.83	J/mol×K	562.30	Joback Method
cpg	515.33	J/mol×K	454.26	Joback Method
cpg	528.52	J/mol×K	475.87	Joback Method
cpg	540.24	J/mol×K	497.48	Joback Method
cpg	550.61	J/mol×K	519.09	Joback Method
cpg	559.76	J/mol×K	540.70	Joback Method
cpg	574.93	J/mol×K	583.91	Joback Method
hvapt	38.60	kJ/mol	323.00	NIST Webbook

Sources

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=C22186647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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