1,2,4,6,7,9-Hexafluoro DBD

Inchi: InChI=1S/C12H2F6O2/c13-3-1-5(15)9-11(7(3)17)20-10-6(16)2-4(14)8(18)12(10)19-9/h1-
InchiKey: FOADTOVERZWUIR-UHFFFAOYSA-N
Formula: C12H2F6O2
SMILES: Fc1cc(F)c2c(c1F)Oc1c(F)cc(F)c(F)c1O2
Mol. weight [g/mol]: 292.13

Physical Properties

Property code	Value	Unit	Source
gf	-1062.60	kJ/mol	Joback Method
hf	-1251.07	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.419		Crippen Method
mcvol	143.920	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	623.82	K	Joback Method
tc	820.08	K	Joback Method
tf	460.38	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.90	J/mol×K	623.82	Joback Method
cpg	367.20	J/mol×K	656.53	Joback Method
cpg	374.98	J/mol×K	689.24	Joback Method
cpg	382.29	J/mol×K	721.95	Joback Method
cpg	389.16	J/mol×K	754.66	Joback Method
cpg	395.61	J/mol×K	787.37	Joback Method
cpg	401.68	J/mol×K	820.08	Joback Method

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=R223962&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
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