Octafluoro DBD

Inchi: InChI=1S/C12F8O2/c13-1-2(14)6(18)10-9(5(1)17)21-11-7(19)3(15)4(16)8(20)12(11)22-1
InchiKey: NNMHAVGAIQTMRH-UHFFFAOYSA-N
Formula: C12F8O2
SMILES: Fc1c(F)c(F)c2c(c1F)Oc1c(F)c(F)c(F)c(F)c1O2
Mol. weight [g/mol]: 328.11

Physical Properties

Property code	Value	Unit	Source
gf	-1471.48	kJ/mol	Joback Method
hf	-1666.23	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	56.01	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.697		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1441.00		NIST Webbook
tb	632.32	K	Joback Method
tc	815.06	K	Joback Method
tf	486.60	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.30	J/mol×K	632.32	Joback Method
cpg	379.52	J/mol×K	662.78	Joback Method
cpg	386.36	J/mol×K	693.23	Joback Method
cpg	392.82	J/mol×K	723.69	Joback Method
cpg	398.93	J/mol×K	754.14	Joback Method
cpg	404.71	J/mol×K	784.60	Joback Method
cpg	410.18	J/mol×K	815.06	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224014&Units=SI

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