1,2,3,4,6-Pentafluoro DBD

Inchi: InChI=1S/C12H3F5O2/c13-4-2-1-3-5-10(4)19-12-9(17)7(15)6(14)8(16)11(12)18-5/h1-3H
InchiKey: JWUZDDGDYPRMLQ-UHFFFAOYSA-N
Formula: C12H3F5O2
SMILES: Fc1cccc2c1Oc1c(F)c(F)c(F)c(F)c1O2
Mol. weight [g/mol]: 274.14

Physical Properties

Property code	Value	Unit	Source
gf	-858.16	kJ/mol	Joback Method
hf	-1043.49	kJ/mol	Joback Method
hfus	42.72	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.280		Crippen Method
mcvol	142.150	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	619.57	K	Joback Method
tc	823.63	K	Joback Method
tf	447.27	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.10	J/mol×K	619.57	Joback Method
cpg	361.01	J/mol×K	653.58	Joback Method
cpg	369.34	J/mol×K	687.59	Joback Method
cpg	377.13	J/mol×K	721.60	Joback Method
cpg	384.42	J/mol×K	755.61	Joback Method
cpg	391.24	J/mol×K	789.62	Joback Method
cpg	397.65	J/mol×K	823.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R223937&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
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