1,6-Difluoro DBD

Inchi: InChI=1S/C12H6F2O2/c13-7-3-1-5-9-11(7)16-10-6-2-4-8(14)12(10)15-9/h1-6H
InchiKey: SUZZELGAHSENSY-UHFFFAOYSA-N
Formula: C12H6F2O2
SMILES: Fc1cccc2c1Oc1cccc(F)c1O2
Mol. weight [g/mol]: 220.17

Physical Properties

Property code	Value	Unit	Source
gf	-244.84	kJ/mol	Joback Method
hf	-420.75	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.863		Crippen Method
mcvol	136.840	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	606.82	K	Joback Method
tc	838.90	K	Joback Method
tf	407.94	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.26	J/mol×K	606.82	Joback Method
cpg	342.42	J/mol×K	645.50	Joback Method
cpg	352.70	J/mol×K	684.18	Joback Method
cpg	362.17	J/mol×K	722.86	Joback Method
cpg	370.91	J/mol×K	761.54	Joback Method
cpg	379.01	J/mol×K	800.22	Joback Method
cpg	386.55	J/mol×K	838.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R223982&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