1,2,6,7-Tetrafluoro-DBD

Inchi: InChI=1S/C12H4F4O2/c13-5-1-3-7-11(9(5)15)18-8-4-2-6(14)10(16)12(8)17-7/h1-4H
InchiKey: NATCITNWZSCRQV-UHFFFAOYSA-N
Formula: C12H4F4O2
SMILES: Fc1ccc2c(c1F)Oc1ccc(F)c(F)c1O2
Mol. weight [g/mol]: 256.15

Physical Properties

Property code	Value	Unit	Source
gf	-653.72	kJ/mol	Joback Method
hf	-835.91	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.141		Crippen Method
mcvol	140.380	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
tb	615.32	K	Joback Method
tc	827.93	K	Joback Method
tf	434.16	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.22	J/mol×K	615.32	Joback Method
cpg	354.82	J/mol×K	650.76	Joback Method
cpg	363.74	J/mol×K	686.19	Joback Method
cpg	372.05	J/mol×K	721.63	Joback Method
cpg	379.79	J/mol×K	757.06	Joback Method
cpg	387.01	J/mol×K	792.50	Joback Method
cpg	393.78	J/mol×K	827.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R223977&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