2,3,4,5,6-Pentafluorobenzhydrol

Inchi: InChI=1S/C13H7F5O/c14-8-7(9(15)11(17)12(18)10(8)16)13(19)6-4-2-1-3-5-6/h1-5,13,19
InchiKey: PMIIFKURPQGSMI-UHFFFAOYSA-N
Formula: C13H7F5O
SMILES: OC(c1ccccc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 274.19
CAS: 27599-16-2

Physical Properties

Property code	Value	Unit	Source
gf	-878.06	kJ/mol	Joback Method
hf	-1034.00	kJ/mol	Joback Method
hfus	31.53	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.464		Crippen Method
mcvol	161.230	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	663.19	K	Joback Method
tc	851.74	K	Joback Method
tf	400.48	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.88	J/mol×K	663.19	Joback Method
cpg	423.82	J/mol×K	694.62	Joback Method
cpg	433.17	J/mol×K	726.04	Joback Method
cpg	441.93	J/mol×K	757.47	Joback Method
cpg	450.14	J/mol×K	788.89	Joback Method
cpg	457.81	J/mol×K	820.32	Joback Method
cpg	464.96	J/mol×K	851.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27599162&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume