3,5-Dihydroxybenzyl alcohol, tris(pentafluoropropionate)

Inchi: InChI=1S/C16H5F15O6/c17-11(18,14(23,24)25)8(32)35-4-5-1-6(36-9(33)12(19,20)15(26
InchiKey: NXGZXCJPXLQXHW-UHFFFAOYSA-N
Formula: C16H5F15O6
SMILES: O=C(OCc1cc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 578.18

Physical Properties

Property code	Value	Unit	Source
gf	-3429.88	kJ/mol	Joback Method
hf	-3888.53	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.133		Crippen Method
mcvol	261.410	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	800.66	K	Joback Method
tc	980.98	K	Joback Method
tf	561.39	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.64	J/mol×K	800.66	Joback Method
cpg	823.01	J/mol×K	830.71	Joback Method
cpg	830.58	J/mol×K	860.77	Joback Method
cpg	837.45	J/mol×K	890.82	Joback Method
cpg	843.67	J/mol×K	920.88	Joback Method
cpg	849.34	J/mol×K	950.93	Joback Method
cpg	854.53	J/mol×K	980.98	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=U376163&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