3,5-Dihydroxybenzyl alcohol, tris(heptafluorobutyrate)

Inchi: InChI=1S/C19H5F21O6/c20-11(21,14(26,27)17(32,33)34)8(41)44-4-5-1-6(45-9(42)12(22

InchiKey: LEMOQPWTCMZOIO-UHFFFAOYSA-N

Formula: C19H5F21O6

SMILES: O=C(OCc1cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1)C(F

Mol. weight [g/mol]: 728.21

Physical Properties

Property code	Value	Unit	Source
gf	-4564.96	kJ/mol	Joback Method
hf	-5153.36	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	60.13	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	7.039		Crippen Method
mcvol	314.300	ml/mol	McGowan Method
pc	876.88	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	855.23	K	Joback Method
tc	1051.94	K	Joback Method
tf	606.00	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.66	J/mol×K	855.23	Joback Method
cpg	1035.18	J/mol×K	888.02	Joback Method
cpg	1042.90	J/mol×K	920.80	Joback Method
cpg	1049.97	J/mol×K	953.59	Joback Method
cpg	1056.56	J/mol×K	986.37	Joback Method
cpg	1062.84	J/mol×K	1019.16	Joback Method
cpg	1068.96	J/mol×K	1051.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376162&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume