3-Hydroxy-4-methoxybenzyl alcohol, di(heptafluorobutyrate)

Inchi: InChI=1S/C16H8F14O5/c1-33-7-3-2-6(5-34-9(31)11(17,18)13(21,22)15(25,26)27)4-8(7)3

InchiKey: DLLXSSJUWWRHSJ-UHFFFAOYSA-N

Formula: C16H8F14O5

SMILES: COc1ccc(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 546.21

Physical Properties

Property code	Value	Unit	Source
gf	-3106.15	kJ/mol	Joback Method
hf	-3579.84	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.310		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	747.52	K	Joback Method
tc	919.23	K	Joback Method
tf	510.87	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.50	J/mol×K	747.52	Joback Method
cpg	806.53	J/mol×K	776.14	Joback Method
cpg	815.74	J/mol×K	804.76	Joback Method
cpg	824.17	J/mol×K	833.37	Joback Method
cpg	831.90	J/mol×K	861.99	Joback Method
cpg	839.00	J/mol×K	890.61	Joback Method
cpg	845.53	J/mol×K	919.23	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=U374855&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