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

Inchi: InChI=1S/C14H8F10O5/c1-27-7-3-2-6(5-28-9(25)11(15,16)13(19,20)21)4-8(7)29-10(26)1

InchiKey: MMBBXEVJTBQMFR-UHFFFAOYSA-N

Formula: C14H8F10O5

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

Mol. weight [g/mol]: 446.19

Physical Properties

Property code	Value	Unit	Source
gf	-2349.43	kJ/mol	Joback Method
hf	-2736.62	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.039		Crippen Method
mcvol	222.810	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1371.00		NIST Webbook
tb	711.14	K	Joback Method
tc	885.68	K	Joback Method
tf	481.13	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.84	J/mol×K	711.14	Joback Method
cpg	665.14	J/mol×K	740.23	Joback Method
cpg	674.65	J/mol×K	769.32	Joback Method
cpg	683.41	J/mol×K	798.41	Joback Method
cpg	691.46	J/mol×K	827.50	Joback Method
cpg	698.85	J/mol×K	856.59	Joback Method
cpg	705.63	J/mol×K	885.68	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=U374854&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

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