2-Hydroxy-5-nitrobenzyl alcohol, bis(pentafluoropropionate)

Inchi: InChI=1S/C13H5F10NO6/c14-10(15,12(18,19)20)8(25)29-4-5-3-6(24(27)28)1-2-7(5)30-9

InchiKey: GICYDGRWESWUQK-UHFFFAOYSA-N

Formula: C13H5F10NO6

SMILES: O=C(OCc1cc([N+](=O)[O-])ccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 461.17

Physical Properties

Property code	Value	Unit	Source
gf	-2217.30	kJ/mol	Joback Method
hf	-2594.52	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	69.68	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	3.939		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	817.68	K	Joback Method
tc	1014.77	K	Joback Method
tf	591.24	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.96	J/mol×K	817.68	Joback Method
cpg	676.63	J/mol×K	850.53	Joback Method
cpg	683.55	J/mol×K	883.38	Joback Method
cpg	689.81	J/mol×K	916.22	Joback Method
cpg	695.47	J/mol×K	949.07	Joback Method
cpg	700.61	J/mol×K	981.92	Joback Method
cpg	705.31	J/mol×K	1014.77	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=U376157&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