5-Bromo-2-hydroxybenzyl alcohol, bis(pentafluoropropionate)

Inchi: InChI=1S/C13H5BrF10O4/c14-6-1-2-7(28-9(26)11(17,18)13(22,23)24)5(3-6)4-27-8(25)10

InchiKey: PFQQFEFDFVAAAY-UHFFFAOYSA-N

Formula: C13H5BrF10O4

SMILES: O=C(OCc1cc(Br)ccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 495.06

Physical Properties

Property code	Value	Unit	Source
gf	-2238.53	kJ/mol	Joback Method
hf	-2557.43	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.793		Crippen Method
mcvol	220.350	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	732.00	K	Joback Method
tc	916.75	K	Joback Method
tf	507.43	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.20	J/mol×K	732.00	Joback Method
cpg	620.74	J/mol×K	762.79	Joback Method
cpg	628.54	J/mol×K	793.58	Joback Method
cpg	635.64	J/mol×K	824.37	Joback Method
cpg	642.11	J/mol×K	855.17	Joback Method
cpg	648.02	J/mol×K	885.96	Joback Method
cpg	653.44	J/mol×K	916.75	Joback Method

Sources

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=U376148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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