2-Hydroxybenzyl alcohol, bis(pentafluoropropionate)

Inchi: InChI=1S/C13H6F10O4/c14-10(15,12(18,19)20)8(24)26-5-6-3-1-2-4-7(6)27-9(25)11(16,1

InchiKey: NJMGLCMOCKABEQ-UHFFFAOYSA-N

Formula: C13H6F10O4

SMILES: O=C(OCc1ccccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 416.17

Physical Properties

Property code	Value	Unit	Source
gf	-2243.22	kJ/mol	Joback Method
hf	-2572.29	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.030		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1154.00		NIST Webbook
tb	660.86	K	Joback Method
tc	833.53	K	Joback Method
tf	435.11	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.03	J/mol×K	660.86	Joback Method
cpg	590.34	J/mol×K	689.64	Joback Method
cpg	599.82	J/mol×K	718.42	Joback Method
cpg	608.53	J/mol×K	747.20	Joback Method
cpg	616.53	J/mol×K	775.97	Joback Method
cpg	623.87	J/mol×K	804.75	Joback Method
cpg	630.59	J/mol×K	833.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376192&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