3,5-Dihydroxybenzyl alcohol, tris(trifluoroacetate)

Inchi: InChI=1S/C13H5F9O6/c14-11(15,16)8(23)26-4-5-1-6(27-9(24)12(17,18)19)3-7(2-5)28-10

InchiKey: FTYDVVMEIZKILN-UHFFFAOYSA-N

Formula: C13H5F9O6

SMILES: O=C(OCc1cc(OC(=O)C(F)(F)F)cc(OC(=O)C(F)(F)F)c1)C(F)(F)F

Mol. weight [g/mol]: 428.16

Physical Properties

Property code	Value	Unit	Source
gf	-2294.80	kJ/mol	Joback Method
hf	-2623.70	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.228		Crippen Method
mcvol	208.520	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	746.09	K	Joback Method
tc	927.59	K	Joback Method
tf	516.78	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.89	J/mol×K	746.09	Joback Method
cpg	612.57	J/mol×K	776.34	Joback Method
cpg	620.52	J/mol×K	806.59	Joback Method
cpg	627.76	J/mol×K	836.84	Joback Method
cpg	634.32	J/mol×K	867.09	Joback Method
cpg	640.25	J/mol×K	897.34	Joback Method
cpg	645.56	J/mol×K	927.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376164&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