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

Inchi: InChI=1S/C11H5F6NO6/c12-10(13,14)8(19)23-4-5-3-6(18(21)22)1-2-7(5)24-9(20)11(15,1

InchiKey: KRUMBDKHYXTJHW-UHFFFAOYSA-N

Formula: C11H5F6NO6

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

Mol. weight [g/mol]: 361.15

Physical Properties

Property code	Value	Unit	Source
gf	-1460.58	kJ/mol	Joback Method
hf	-1751.30	kJ/mol	Joback Method
hfus	38.10	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	2.668		Crippen Method
mcvol	185.010	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	781.30	K	Joback Method
tc	988.61	K	Joback Method
tf	561.50	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.59	J/mol×K	781.30	Joback Method
cpg	537.73	J/mol×K	815.85	Joback Method
cpg	545.08	J/mol×K	850.40	Joback Method
cpg	551.69	J/mol×K	884.95	Joback Method
cpg	557.60	J/mol×K	919.51	Joback Method
cpg	562.84	J/mol×K	954.06	Joback Method
cpg	567.46	J/mol×K	988.61	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=U376158&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