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

Inchi: InChI=1S/C11H5BrF6O4/c12-6-1-2-7(22-9(20)11(16,17)18)5(3-6)4-21-8(19)10(13,14)15/

InchiKey: AAWFKQZMAFIGMQ-UHFFFAOYSA-N

Formula: C11H5BrF6O4

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

Mol. weight [g/mol]: 395.05

Physical Properties

Property code	Value	Unit	Source
gf	-1481.81	kJ/mol	Joback Method
hf	-1714.21	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	60.93	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.522		Crippen Method
mcvol	185.090	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1333.00		NIST Webbook
tb	695.62	K	Joback Method
tc	892.42	K	Joback Method
tf	477.69	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.11	J/mol×K	695.62	Joback Method
cpg	482.91	J/mol×K	728.42	Joback Method
cpg	490.99	J/mol×K	761.22	Joback Method
cpg	498.39	J/mol×K	794.02	Joback Method
cpg	505.15	J/mol×K	826.82	Joback Method
cpg	511.30	J/mol×K	859.62	Joback Method
cpg	516.88	J/mol×K	892.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376149&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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