2-Hydroxybenzyl alcohol, bis(trifluoroacetate)

Inchi: InChI=1S/C11H6F6O4/c12-10(13,14)8(18)20-5-6-3-1-2-4-7(6)21-9(19)11(15,16)17/h1-4H
InchiKey: USPRDSFGAWCQMY-UHFFFAOYSA-N
Formula: C11H6F6O4
SMILES: O=C(OCc1ccccc1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 316.15

Physical Properties

Property code	Value	Unit	Source
gf	-1486.50	kJ/mol	Joback Method
hf	-1729.07	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	53.84	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.760		Crippen Method
mcvol	167.590	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
tb	624.48	K	Joback Method
tc	809.32	K	Joback Method
tf	405.37	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.65	J/mol×K	624.48	Joback Method
cpg	453.00	J/mol×K	655.29	Joback Method
cpg	462.62	J/mol×K	686.09	Joback Method
cpg	471.54	J/mol×K	716.90	Joback Method
cpg	479.78	J/mol×K	747.71	Joback Method
cpg	487.37	J/mol×K	778.52	Joback Method
cpg	494.35	J/mol×K	809.32	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=U376193&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

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