4-Hydroxy-3-methoxybenzyl alcohol, bis(trifluoroacetate)

Inchi: InChI=1S/C12H8F6O5/c1-21-8-4-6(5-22-9(19)11(13,14)15)2-3-7(8)23-10(20)12(16,17)18

InchiKey: PDIASPQUSUCDCN-UHFFFAOYSA-N

Formula: C12H8F6O5

SMILES: COc1cc(COC(=O)C(F)(F)F)ccc1OC(=O)C(F)(F)F

Mol. weight [g/mol]: 346.18

Physical Properties

Property code	Value	Unit	Source
gf	-1592.71	kJ/mol	Joback Method
hf	-1893.40	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.768		Crippen Method
mcvol	187.550	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
tb	674.76	K	Joback Method
tc	858.51	K	Joback Method
tf	451.39	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.84	J/mol×K	674.76	Joback Method
cpg	525.37	J/mol×K	705.38	Joback Method
cpg	535.19	J/mol×K	736.01	Joback Method
cpg	544.30	J/mol×K	766.63	Joback Method
cpg	552.74	J/mol×K	797.26	Joback Method
cpg	560.51	J/mol×K	827.88	Joback Method
cpg	567.64	J/mol×K	858.51	Joback Method

Sources

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=U376173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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