3,4-dihydroxymandelic acid, TFA-ME

Inchi: InChI=1S/C15H7F9O8/c1-29-9(25)8(32-12(28)15(22,23)24)5-2-3-6(30-10(26)13(16,17)1
InchiKey: JQBMUKVTPUXGJQ-UHFFFAOYSA-N
Formula: C15H7F9O8
SMILES: COC(=O)C(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 486.20

Physical Properties

Property code	Value	Unit	Source
gf	-2514.32	kJ/mol	Joback Method
hf	-2915.06	kJ/mol	Joback Method
hfus	40.97	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	2.942		Crippen Method
mcvol	244.140	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
tb	867.70	K	Joback Method
tc	1064.98	K	Joback Method
tf	596.48	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.51	J/mol×K	867.70	Joback Method
cpg	749.26	J/mol×K	900.58	Joback Method
cpg	756.08	J/mol×K	933.46	Joback Method
cpg	762.03	J/mol×K	966.34	Joback Method
cpg	767.13	J/mol×K	999.22	Joback Method
cpg	771.41	J/mol×K	1032.10	Joback Method
cpg	774.91	J/mol×K	1064.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387150&Units=SI

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