Mandelic acid, 3,4-dihydroxy, DCTFA-acetate

Inchi: InChI=1S/C15H10Cl2F4O7/c1-6(22)25-9-4-3-8(5-10(9)26-7(2)23)11-12(24)28-13(27-11,1

InchiKey: LTHCVEVXKXZLQD-UHFFFAOYSA-N

Formula: C15H10Cl2F4O7

SMILES: CC(=O)Oc1ccc(C2OC(C(F)(F)Cl)(C(F)(F)Cl)OC2=O)cc1OC(C)=O

Mol. weight [g/mol]: 449.13

Physical Properties

Property code	Value	Unit	Source
gf	-1368.17	kJ/mol	Joback Method
hf	-1808.68	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.511		Crippen Method
mcvol	247.340	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
tb	929.87	K	Joback Method
tc	1164.01	K	Joback Method
tf	673.55	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.74	J/mol×K	929.87	Joback Method
cpg	757.62	J/mol×K	968.89	Joback Method
cpg	769.16	J/mol×K	1007.92	Joback Method
cpg	780.49	J/mol×K	1046.94	Joback Method
cpg	791.74	J/mol×K	1085.96	Joback Method
cpg	803.06	J/mol×K	1124.99	Joback Method
cpg	814.57	J/mol×K	1164.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57694&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