Mandelic acid, 3-hydroxy, DCTFA-acetate

Inchi: InChI=1S/C13H8Cl2F4O5/c1-6(20)22-8-4-2-3-7(5-8)9-10(21)24-11(23-9,12(14,16)17)13(
InchiKey: NFIKAKAFHSSFLW-UHFFFAOYSA-N
Formula: C13H8Cl2F4O5
SMILES: CC(=O)Oc1cccc(C2OC(C(F)(F)Cl)(C(F)(F)Cl)OC2=O)c1
Mol. weight [g/mol]: 391.10

Physical Properties

Property code	Value	Unit	Source
gf	-1141.46	kJ/mol	Joback Method
hf	-1511.13	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.586		Crippen Method
mcvol	211.720	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1739.00		NIST Webbook
tb	802.84	K	Joback Method
tc	1038.43	K	Joback Method
tf	566.33	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.07	J/mol×K	802.84	Joback Method
cpg	615.03	J/mol×K	842.11	Joback Method
cpg	626.45	J/mol×K	881.37	Joback Method
cpg	637.46	J/mol×K	920.64	Joback Method
cpg	648.25	J/mol×K	959.90	Joback Method
cpg	658.95	J/mol×K	999.17	Joback Method
cpg	669.75	J/mol×K	1038.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57701&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

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