2,4,6-Trimethylmandelic acid

Inchi: InChI=1S/C11H14O3/c1-6-4-7(2)9(8(3)5-6)10(12)11(13)14/h4-5,10,12H,1-3H3,(H,13,14)
InchiKey: IRQXVXUXARGLQG-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: Cc1cc(C)c(C(O)C(=O)O)c(C)c1
Mol. weight [g/mol]: 194.23
CAS: 20797-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-279.74	kJ/mol	Joback Method
hf	-490.57	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.730		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	730.49	K	Joback Method
tc	924.78	K	Joback Method
tf	434.28	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.11	J/mol×K	730.49	Joback Method
cpg	430.83	J/mol×K	762.87	Joback Method
cpg	439.99	J/mol×K	795.25	Joback Method
cpg	448.61	J/mol×K	827.63	Joback Method
cpg	456.71	J/mol×K	860.01	Joback Method
cpg	464.30	J/mol×K	892.39	Joback Method
cpg	471.40	J/mol×K	924.78	Joback Method

dvisc	0.0011981	Pa×s	434.28	Joback Method
dvisc	0.0003744	Pa×s	483.65	Joback Method
dvisc	0.0001451	Pa×s	533.02	Joback Method
dvisc	0.0000661	Pa×s	582.38	Joback Method
dvisc	0.0000340	Pa×s	631.75	Joback Method
dvisc	0.0000193	Pa×s	681.12	Joback Method
dvisc	0.0000118	Pa×s	730.49	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=C20797562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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