Melissic acid

Inchi: InChI=1S/C31H62O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24
InchiKey: ONLMUMPTRGEPCH-UHFFFAOYSA-N
Formula: C31H62O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 466.82
CAS: 38232-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-55.60	kJ/mol	Joback Method
hf	-947.98	kJ/mol	Joback Method
hfus	81.73	kJ/mol	Joback Method
hvap	108.02	kJ/mol	Joback Method
log10ws	-11.90		Crippen Method
logp	11.404		Crippen Method
mcvol	455.090	ml/mol	McGowan Method
pc	612.99	kPa	Joback Method
tb	1054.73	K	Joback Method
tc	1352.18	K	Joback Method
tf	549.88	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1661.91	J/mol×K	1054.73	Joback Method
cpg	1691.32	J/mol×K	1104.31	Joback Method
cpg	1718.35	J/mol×K	1153.88	Joback Method
cpg	1743.24	J/mol×K	1203.46	Joback Method
cpg	1766.27	J/mol×K	1253.03	Joback Method
cpg	1787.69	J/mol×K	1302.61	Joback Method
cpg	1807.76	J/mol×K	1352.18	Joback Method
dvisc	0.0002024	Pa×s	549.88	Joback Method
dvisc	0.0000578	Pa×s	634.02	Joback Method

dvisc	0.0000221	Pa×s	718.16	Joback Method
dvisc	0.0000104	Pa×s	802.30	Joback Method
dvisc	0.0000056	Pa×s	886.45	Joback Method
dvisc	0.0000034	Pa×s	970.59	Joback Method
dvisc	0.0000022	Pa×s	1054.73	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=C38232018&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume