

Glutaric acid, (2-methylcyclohex-1-enyl)methyl

InChI: InChI=1S/C19H32O4/c1-5-17(14(2)3)23-19(21)12-8-11-18(20)22-13-16-10-7-6-9-15(16)
InChIKey: DTOFYLGVDMAUSC-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCC(OC(=O)CCCC(=O)OCC1=C(C)CCCC1)C(C)C

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-320.76	kJ/mol	Joback Method
hf	-826.15	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.568		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinqol	2174.00		NIST Webbook
tb	819.16	K	Joback Method
tc	1021.06	K	Joback Method
tf	455.63	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.45	J/molxK	819.16	Joback Method
cpg	952.16	J/molxK	987.41	Joback Method
cpg	939.22	J/molxK	953.76	Joback Method
cpg	925.10	J/molxK	920.11	Joback Method
cpg	909.77	J/molxK	886.46	Joback Method
cpg	893.23	J/molxK	852.81	Joback Method
cpg	963.94	J/molxK	1021.06	Joback Method
dvisc	0.0000458	Paxs	819.16	Joback Method
dvisc	0.0000619	Paxs	758.57	Joback Method

dvisc	0.0000882	Paxs	697.98	Joback Method
dvisc	0.0001342	Paxs	637.39	Joback Method
dvisc	0.0002231	Paxs	576.81	Joback Method
dvisc	0.0004180	Paxs	516.22	Joback Method
dvisc	0.0009255	Paxs	455.63	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=U405503&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

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