

Glutaric acid, myrtenyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C20H32O4/c1-13(2)14(3)24-19(22)8-6-7-18(21)23-12-15-9-10-16-11-17(15)20
InchiKey: IJSKQCHCEDUKJI-UHFFFAOYSA-N
Formula: C20H32O4
SMILES: CC(C)C(C)OC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-238.67	kJ/mol	Joback Method
hf	-775.64	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	77.14	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.280		Crippen Method
mvol	281.520	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	826.16	K	Joback Method
tc	1030.51	K	Joback Method
tf	494.78	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.77	J/mol×K	826.16	Joback Method
cpg	933.29	J/mol×K	860.22	Joback Method
cpg	952.19	J/mol×K	894.28	Joback Method
cpg	970.58	J/mol×K	928.33	Joback Method
cpg	988.58	J/mol×K	962.39	Joback Method
cpg	1006.32	J/mol×K	996.45	Joback Method
cpg	1023.93	J/mol×K	1030.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405538&Units=SI

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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