Glutaric acid, 3,4-dimethylcyclohexyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C18H32O4/c1-12(2)15(5)21-17(19)7-6-8-18(20)22-16-10-9-13(3)14(4)11-16/h1

InchiKey: QOZNEYQQEDLVKI-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)OC1CCC(C)C(C)C1

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-363.01	kJ/mol	Joback Method
hf	-901.37	kJ/mol	Joback Method
hfus	34.88	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.112		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	773.15	K	Joback Method
tc	972.02	K	Joback Method
tf	405.84	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.44	J/mol×K	773.15	Joback Method
cpg	872.38	J/mol×K	806.30	Joback Method
cpg	890.99	J/mol×K	839.44	Joback Method
cpg	908.27	J/mol×K	872.59	Joback Method
cpg	924.24	J/mol×K	905.73	Joback Method
cpg	938.88	J/mol×K	938.88	Joback Method
cpg	952.23	J/mol×K	972.02	Joback Method
dvisc	0.0017284	Pa×s	405.84	Joback Method

dvisc	0.0007844	Pa×s	467.06	Joback Method
dvisc	0.0004275	Pa×s	528.28	Joback Method
dvisc	0.0002643	Pa×s	589.50	Joback Method
dvisc	0.0001788	Pa×s	650.71	Joback Method
dvisc	0.0001294	Pa×s	711.93	Joback Method
dvisc	0.0000986	Pa×s	773.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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