Glutaric acid, isobutyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C13H22O5/c1-9(2)8-17-12(15)6-5-7-13(16)18-11(4)10(3)14/h9,11H,5-8H2,1-4
InchiKey: QYJTZJKDGFPZIV-UHFFFAOYSA-N
Formula: C13H22O5
SMILES: CC(=O)C(C)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]: 258.31

Physical Properties

Property code	Value	Unit	Source
gf	-543.06	kJ/mol	Joback Method
hf	-924.39	kJ/mol	Joback Method
hfus	29.55	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.877		Crippen Method
mcvol	210.480	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1730.00		NIST Webbook
tb	702.41	K	Joback Method
tc	891.53	K	Joback Method
tf	400.52	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.37	J/mol×K	702.41	Joback Method
cpg	654.61	J/mol×K	860.01	Joback Method
cpg	643.34	J/mol×K	828.49	Joback Method
cpg	631.29	J/mol×K	796.97	Joback Method
cpg	618.44	J/mol×K	765.45	Joback Method
cpg	604.80	J/mol×K	733.93	Joback Method
cpg	665.09	J/mol×K	891.53	Joback Method
dvisc	0.0001143	Pa×s	702.41	Joback Method
dvisc	0.0001520	Pa×s	652.10	Joback Method

dvisc	0.0002120	Pa×s	601.78	Joback Method
dvisc	0.0003140	Pa×s	551.47	Joback Method
dvisc	0.0005035	Pa×s	501.15	Joback Method
dvisc	0.0008970	Pa×s	450.83	Joback Method
dvisc	0.0018474	Pa×s	400.52	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U359702&Units=SI

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