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

Inchi: InChI=1S/C13H22O5/c1-4-5-9-17-12(15)7-6-8-13(16)18-11(3)10(2)14/h11H,4-9H2,1-3H3
InchiKey: BUSJEQYJLDIKCC-UHFFFAOYSA-N
Formula: C13H22O5
SMILES: CCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 258.31

Physical Properties

Property code	Value	Unit	Source
gf	-540.62	kJ/mol	Joback Method
hf	-919.11	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.021		Crippen Method
mcvol	210.480	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	1774.00		NIST Webbook
tb	702.85	K	Joback Method
tc	889.34	K	Joback Method
tf	415.52	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.85	J/mol×K	702.85	Joback Method
cpg	604.06	J/mol×K	733.93	Joback Method
cpg	617.50	J/mol×K	765.01	Joback Method
cpg	630.19	J/mol×K	796.10	Joback Method
cpg	642.12	J/mol×K	827.18	Joback Method
cpg	653.28	J/mol×K	858.26	Joback Method
cpg	663.69	J/mol×K	889.34	Joback Method
dvisc	0.0015266	Pa×s	415.52	Joback Method
dvisc	0.0008087	Pa×s	463.41	Joback Method

dvisc	0.0004825	Pa×s	511.30	Joback Method
dvisc	0.0003145	Pa×s	559.18	Joback Method
dvisc	0.0002193	Pa×s	607.07	Joback Method
dvisc	0.0001612	Pa×s	654.96	Joback Method
dvisc	0.0001236	Pa×s	702.85	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=U359703&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