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

Inchi: InChI=1S/C15H26O5/c1-11(2)7-6-10-19-14(17)8-5-9-15(18)20-13(4)12(3)16/h11,13H,5-1
InchiKey: MCTLURRWPDIDQC-UHFFFAOYSA-N
Formula: C15H26O5
SMILES: CC(=O)C(C)OC(=O)CCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 286.36

Physical Properties

Property code	Value	Unit	Source
gf	-526.22	kJ/mol	Joback Method
hf	-965.67	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.657		Crippen Method
mcvol	238.660	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	748.17	K	Joback Method
tc	936.03	K	Joback Method
tf	423.06	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.46	J/mol×K	748.17	Joback Method
cpg	715.70	J/mol×K	779.48	Joback Method
cpg	730.06	J/mol×K	810.79	Joback Method
cpg	743.54	J/mol×K	842.10	Joback Method
cpg	756.15	J/mol×K	873.41	Joback Method
cpg	767.89	J/mol×K	904.72	Joback Method
cpg	778.77	J/mol×K	936.03	Joback Method
dvisc	0.0015206	Pa×s	423.06	Joback Method

dvisc	0.0007209	Pa×s	477.25	Joback Method
dvisc	0.0003979	Pa×s	531.43	Joback Method
dvisc	0.0002452	Pa×s	585.62	Joback Method
dvisc	0.0001640	Pa×s	639.80	Joback Method
dvisc	0.0001168	Pa×s	693.98	Joback Method
dvisc	0.0000874	Pa×s	748.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359705&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

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