

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

Inchi: InChI=1S/C15H26O5/c1-4-5-6-7-11-19-14(17)9-8-10-15(18)20-13(3)12(2)16/h13H,4-11H
InchiKey: HYVVSODHXKSSPQ-UHFFFAOYSA-N
Formula: C15H26O5
SMILES: CCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 286.36

Physical Properties

Property code	Value	Unit	Source
gf	-523.78	kJ/mol	Joback Method
hf	-960.39	kJ/mol	Joback Method
hfus	38.26	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.801		Crippen Method
mcvol	238.660	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1971.00		NIST Webbook
tb	748.61	K	Joback Method
tc	934.38	K	Joback Method
tf	438.06	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.93	J/mol×K	748.61	Joback Method
cpg	715.00	J/mol×K	779.57	Joback Method
cpg	729.20	J/mol×K	810.53	Joback Method
cpg	742.56	J/mol×K	841.50	Joback Method
cpg	755.07	J/mol×K	872.46	Joback Method
cpg	766.74	J/mol×K	903.42	Joback Method
cpg	777.57	J/mol×K	934.38	Joback Method
dvisc	0.0012734	Pa×s	438.06	Joback Method
dvisc	0.0006570	Pa×s	489.82	Joback Method

dvisc	0.0003847	Pa×s	541.58	Joback Method
dvisc	0.0002473	Pa×s	593.34	Joback Method
dvisc	0.0001706	Pa×s	645.09	Joback Method
dvisc	0.0001244	Pa×s	696.85	Joback Method
dvisc	0.0000948	Pa×s	748.61	Joback Method

Sources

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=U359706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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