

Glutaric acid, isobutyl 5-methoxy-3-methylpent-2-yl ester

Inchi:	InChI=1S/C16H30O5/c1-12(2)11-20-15(17)7-6-8-16(18)21-14(4)13(3)9-10-19-5/h12-14H
InchiKey:	ZURSDWSLCIXXBH-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	COCCC(C)C(C)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-496.32	kJ/mol	Joback Method
hf	-1011.23	kJ/mol	Joback Method
hfus	33.39	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.960		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinqol	1960.00		NIST Webbook
tb	739.16	K	Joback Method
tc	922.02	K	Joback Method
tf	391.63	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.12	J/molxK	739.16	Joback Method
cpg	782.03	J/molxK	769.64	Joback Method
cpg	798.01	J/molxK	800.11	Joback Method
cpg	813.08	J/molxK	830.59	Joback Method
cpg	827.22	J/molxK	861.06	Joback Method
cpg	840.43	J/molxK	891.54	Joback Method
cpg	852.72	J/molxK	922.02	Joback Method
dvisc	0.0015736	Paxs	391.63	Joback Method
dvisc	0.0006286	Paxs	449.55	Joback Method

dvisc	0.0003096	Paxs	507.47	Joback Method
dvisc	0.0001763	Paxs	565.39	Joback Method
dvisc	0.0001115	Paxs	623.32	Joback Method
dvisc	0.0000762	Paxs	681.24	Joback Method
dvisc	0.0000553	Paxs	739.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U358432&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

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