

di-(1-Methyl-2-methoxybutyl)glutarate

Inchi:	InChI=1S/C15H28O6/c1-10(18-5)12(3)20-14(16)8-7-9-15(17)21-13(4)11(2)19-6/h10-13H
InchiKey:	WADRIZWFKOCMFR-UHFFFAOYSA-N
Formula:	C15H28O6
SMILES:	COC(C)C(C)OC(=O)CCCC(=O)OC(C)C(C)OC
Mol. weight [g/mol]:	304.38

Physical Properties

Property code	Value	Unit	Source
gf	-612.18	kJ/mol	Joback Method
hf	-1128.09	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.090		Crippen Method
mcvol	248.830	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1684.00		NIST Webbook
tb	738.26	K	Joback Method
tc	923.66	K	Joback Method
tf	387.59	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.27	J/molxK	738.26	Joback Method
cpg	754.75	J/molxK	769.16	Joback Method
cpg	770.29	J/molxK	800.06	Joback Method
cpg	784.88	J/molxK	830.96	Joback Method
cpg	798.52	J/molxK	861.86	Joback Method
cpg	811.18	J/molxK	892.76	Joback Method
cpg	822.85	J/molxK	923.66	Joback Method
dvisc	0.0014663	Paxs	387.59	Joback Method
dvisc	0.0005585	Paxs	446.04	Joback Method

dvisc	0.0002661	Paxs	504.48	Joback Method
dvisc	0.0001479	Paxs	562.92	Joback Method
dvisc	0.0000918	Paxs	621.37	Joback Method
dvisc	0.0000618	Paxs	679.82	Joback Method
dvisc	0.0000443	Paxs	738.26	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=R541834&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

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