

Glutaric acid, 3-methylbut-2-yl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C16H30O4/c1-7-14(12(4)5)20-16(18)10-8-9-15(17)19-13(6)11(2)3/h11-14H,7-
InchiKey:	DDSJLMZLUBZRMM-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OC(C)C(C)C)C(C)C
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-393.76	kJ/mol	Joback Method
hf	-884.29	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.722		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	716.30	K	Joback Method
tc	900.82	K	Joback Method
tf	354.40	K	Joback Method
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.52	J/molxK	716.30	Joback Method
cpg	752.94	J/molxK	747.05	Joback Method
cpg	769.44	J/molxK	777.81	Joback Method
cpg	785.03	J/molxK	808.56	Joback Method
cpg	799.71	J/molxK	839.31	Joback Method
cpg	813.48	J/molxK	870.06	Joback Method
cpg	826.37	J/molxK	900.82	Joback Method
dvisc	0.0031943	Paxs	354.40	Joback Method

dvisc	0.0010527	Paxs	414.72	Joback Method
dvisc	0.0004599	Paxs	475.03	Joback Method
dvisc	0.0002421	Paxs	535.35	Joback Method
dvisc	0.0001452	Paxs	595.67	Joback Method
dvisc	0.0000956	Paxs	655.98	Joback Method
dvisc	0.0000676	Paxs	716.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393493&Units=SI
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

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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