

Glutaric acid, di(3,3-dimethylbut-2-yl) ester

Inchi: InChI=1S/C17H32O4/c1-12(16(3,4)5)20-14(18)10-9-11-15(19)21-13(2)17(6,7)8/h12-13H
InchiKey: UOKCSQAAEINRQD-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CC(OC(=O)CCCC(=O)OC(C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-374.78	kJ/mol	Joback Method
hf	-911.87	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.112		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	1832.00		NIST Webbook
tb	733.60	K	Joback Method
tc	926.15	K	Joback Method
tf	400.51	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.70	J/mol×K	733.60	Joback Method
cpg	875.46	J/mol×K	894.06	Joback Method
cpg	861.48	J/mol×K	861.97	Joback Method
cpg	846.55	J/mol×K	829.88	Joback Method
cpg	830.64	J/mol×K	797.78	Joback Method
cpg	813.70	J/mol×K	765.69	Joback Method
cpg	888.54	J/mol×K	926.15	Joback Method
dvisc	0.0000472	Pa×s	733.60	Joback Method
dvisc	0.0000675	Pa×s	678.09	Joback Method

dvisc	0.0001028	Pa×s	622.57	Joback Method
dvisc	0.0001702	Pa×s	567.06	Joback Method
dvisc	0.0003142	Pa×s	511.54	Joback Method
dvisc	0.0006736	Pa×s	456.02	Joback Method
dvisc	0.0017841	Pa×s	400.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359764&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

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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