Pentanedioic acid, 3,3-dimethyl-, dimethyl ester

Other names: Glutaric acid, 3,3-dimethyl-, dimethyl ester
Methyl 3,3-dimethylglutarate

Inchi: InChI=1S/C9H16O4/c1-9(2,5-7(10)12-3)6-8(11)13-4/h5-6H2,1-4H3

InchiKey: NPEAPWIQJBAJIO-UHFFFAOYSA-N

Formula: C9H16O4

SMILES: COC(=O)CC(C)(C)CC(=O)OC

Mol. weight [g/mol]: 188.22

CAS: 19184-67-9

Physical Properties

Property code	Value	Unit	Source
gf	-440.10	kJ/mol	Joback Method
hf	-727.44	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.139		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	554.67	K	Joback Method
tc	746.71	K	Joback Method
tf	337.93	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.44	J/mol×K	554.67	Joback Method
cpg	430.80	J/mol×K	714.70	Joback Method
cpg	420.16	J/mol×K	682.69	Joback Method
cpg	408.91	J/mol×K	650.69	Joback Method
cpg	397.05	J/mol×K	618.68	Joback Method
cpg	384.56	J/mol×K	586.68	Joback Method
cpg	440.85	J/mol×K	746.71	Joback Method

dvisc	0.0001927	Pa×s	554.67	Joback Method
dvisc	0.0002520	Pa×s	518.55	Joback Method
dvisc	0.0003430	Pa×s	482.42	Joback Method
dvisc	0.0004907	Pa×s	446.30	Joback Method
dvisc	0.0007478	Pa×s	410.18	Joback Method
dvisc	0.0012362	Pa×s	374.05	Joback Method
dvisc	0.0022755	Pa×s	337.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	2.00	NIST Webbook

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=C19184679&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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