Hexanedioic acid, 3-methyl-, dimethyl ester

Other names: Dimethyl 3-methylhexanedioate
3-Methyl-hexanedioic acid dimethyl ester
Inchi: InChI=1S/C9H16O4/c1-7(6-9(11)13-3)4-5-8(10)12-2/h7H,4-6H2,1-3H3
InchiKey: HOUQYONBQJFBPF-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: COC(=O)CCC(C)CC(=O)OC
Mol. weight [g/mol]: 188.22
CAS: 54576-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-445.38	kJ/mol	Joback Method
hf	-723.97	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.139		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	557.46	K	Joback Method
tc	742.78	K	Joback Method
tf	320.51	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.40	J/mol×K	557.46	Joback Method
cpg	426.64	J/mol×K	711.90	Joback Method
cpg	416.03	J/mol×K	681.01	Joback Method
cpg	404.90	J/mol×K	650.12	Joback Method

cpg	393.25	J/mol×K	619.23	Joback Method
cpg	381.08	J/mol×K	588.35	Joback Method
cpg	436.72	J/mol×K	742.78	Joback Method
dvisc	0.0001960	Pa×s	557.46	Joback Method
dvisc	0.0002553	Pa×s	517.97	Joback Method
dvisc	0.0003474	Pa×s	478.48	Joback Method
dvisc	0.0004996	Pa×s	438.99	Joback Method
dvisc	0.0007719	Pa×s	399.49	Joback Method
dvisc	0.0013123	Pa×s	360.00	Joback Method
dvisc	0.0025423	Pa×s	320.51	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54576135&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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