4-Heptenoic acid, 3,3-dimethyl-6-oxo-, methyl ester

Other names: Methyl (4E)-3,3-dimethyl-6-oxo-4-heptenoate
Inchi: InChI=1S/C10H16O3/c1-8(11)5-6-10(2,3)7-9(12)13-4/h5-6H,7H2,1-4H3/b6-5+
InchiKey: DSMOCXGKAYMOCG-AATRIKPKSA-N
Formula: C10H16O3
SMILES: COC(=O)CC(C)(C)C=CC(C)=O
Mol. weight [g/mol]: 184.23
CAS: 89722-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-246.46	kJ/mol	Joback Method
hf	-498.64	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.721		Crippen Method
mcvol	156.470	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	559.29	K	Joback Method
tc	758.53	K	Joback Method
tf	321.89	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.46	J/mol×K	559.29	Joback Method
cpg	435.30	J/mol×K	725.32	Joback Method
cpg	424.56	J/mol×K	692.11	Joback Method
cpg	413.13	J/mol×K	658.91	Joback Method
cpg	401.00	J/mol×K	625.70	Joback Method
cpg	388.12	J/mol×K	592.50	Joback Method

cpg	445.40	J/mol×K	758.53	Joback Method
dvisc	0.0001843	Pa×s	559.29	Joback Method
dvisc	0.0002447	Pa×s	519.72	Joback Method
dvisc	0.0003405	Pa×s	480.16	Joback Method
dvisc	0.0005028	Pa×s	440.59	Joback Method
dvisc	0.0008016	Pa×s	401.02	Joback Method
dvisc	0.0014156	Pa×s	361.46	Joback Method
dvisc	0.0028749	Pa×s	321.89	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=C89722214&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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