Methyl 6-methyloctanoate

Other names:	Octanoic acid, 6-methyl, methyl ester
	5-Methyl-heptanecarboxylicacidmethylester
Inchi:	InChI=1S/C10H20O2/c1-4-9(2)7-5-6-8-10(11)12-3/h9H,4-8H2,1-3H3
InchiKey:	MMQPDXPEMSYPFH-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCC(C)CCCCC(=O)OC
Mol. weight [g/mol]:	172.26
CAS:	5129-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-203.04	kJ/mol	Joback Method
hf	-499.81	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1188.90		NIST Webbook
rinpol	1188.90		NIST Webbook
ripol	1482.00		NIST Webbook
tb	504.05	K	Joback Method
tc	679.81	K	Joback Method
tf	259.62	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/mol×K	504.05	Joback Method
cpg	382.82	J/mol×K	533.34	Joback Method
cpg	396.77	J/mol×K	562.64	Joback Method

cpg	410.17	J/mol×K	591.93	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
dvisc	0.0046674	Pa×s	259.62	Joback Method
dvisc	0.0019627	Pa×s	300.36	Joback Method
dvisc	0.0010151	Pa×s	341.10	Joback Method
dvisc	0.0006043	Pa×s	381.84	Joback Method
dvisc	0.0003976	Pa×s	422.57	Joback Method
dvisc	0.0002816	Pa×s	463.31	Joback Method
dvisc	0.0002109	Pa×s	504.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129624&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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