

methyl 5-acetoxyhexanoate

Other names:	Methyl hexanoate, 5-acetoxy
Inchi:	InChI=1S/C9H16O4/c1-7(13-8(2)10)5-4-6-9(11)12-3/h7H,4-6H2,1-3H3
InchiKey:	XZGQJRXRXYNRI-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	<chem>COC(=O)CCCC(C)OC(C)=O</chem>
Mol. weight [g/mol]:	188.22
CAS:	35234-22-1

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	-1.43		Crippen Method
logp	1.281		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1759.00		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/molxK	557.46	Joback Method

cpg	381.08	J/mol×K	588.35	Joback Method
cpg	393.25	J/mol×K	619.23	Joback Method
cpg	404.90	J/mol×K	650.12	Joback Method
cpg	416.03	J/mol×K	681.01	Joback Method
cpg	426.64	J/mol×K	711.90	Joback Method
cpg	436.72	J/mol×K	742.78	Joback Method
dvisc	0.0025423	Paxs	320.51	Joback Method
dvisc	0.0013123	Paxs	360.00	Joback Method
dvisc	0.0007719	Paxs	399.49	Joback Method
dvisc	0.0004996	Paxs	438.99	Joback Method
dvisc	0.0003474	Paxs	478.48	Joback Method
dvisc	0.0002553	Paxs	517.97	Joback Method
dvisc	0.0001960	Paxs	557.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C35234221&Units=SI

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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