

methyl 3-acetoxy-2-methylbutanoate

Other names:	methyl 3-acetoxy-2-methylbutyrate
Inchi:	InChI=1S/C8H14O4/c1-5(8(10)11-4)6(2)12-7(3)9/h5-6H,1-4H3
InchiKey:	UYUNIPJXXCRQBO-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	<chem>COC(=O)C(C)C(C)OC(C)=O</chem>
Mol. weight [g/mol]:	174.19

Physical Properties

Property code	Value	Unit	Source
gf	-456.24	kJ/mol	Joback Method
hf	-708.61	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.747		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1554.00		NIST Webbook
tb	534.14	K	Joback Method
tc	725.42	K	Joback Method
tf	294.24	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.86	J/molxK	534.14	Joback Method
cpg	378.34	J/molxK	693.54	Joback Method
cpg	368.23	J/molxK	661.66	Joback Method
cpg	357.62	J/molxK	629.78	Joback Method

cpg	346.52	J/molxK	597.90	Joback Method
cpg	334.93	J/molxK	566.02	Joback Method
cpg	387.93	J/molxK	725.42	Joback Method
dvisc	0.0002027	Paxs	534.14	Joback Method
dvisc	0.0002693	Paxs	494.16	Joback Method
dvisc	0.0003762	Paxs	454.17	Joback Method
dvisc	0.0005605	Paxs	414.19	Joback Method
dvisc	0.0009094	Paxs	374.21	Joback Method
dvisc	0.0016565	Paxs	334.22	Joback Method
dvisc	0.0035516	Paxs	294.24	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=R319503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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