

methyl 4-acetoxyoctanoate

Inchi:	InChI=1S/C11H20O4/c1-4-5-6-10(15-9(2)12)7-8-11(13)14-3/h10H,4-8H2,1-3H3
InchiKey:	USUFETQYKYBUHJ-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCCCC(CCC(=O)OC)OC(C)=O
Mol. weight [g/mol]:	216.27

Physical Properties

Property code	Value	Unit	Source
gf	-428.54	kJ/mol	Joback Method
hf	-765.25	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.062		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1379.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1381.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1855.00		NIST Webbook
tb	603.22	K	Joback Method
tc	784.89	K	Joback Method
tf	343.05	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.43	J/molxK	603.22	Joback Method

cpg	479.63	J/mol×K	633.50	Joback Method
cpg	493.21	J/mol×K	663.78	Joback Method
cpg	506.18	J/mol×K	694.06	Joback Method
cpg	518.53	J/mol×K	724.34	Joback Method
cpg	530.27	J/mol×K	754.61	Joback Method
cpg	541.38	J/mol×K	784.89	Joback Method
dvisc	0.0022861	Paxs	343.05	Joback Method
dvisc	0.0011425	Paxs	386.41	Joback Method
dvisc	0.0006567	Paxs	429.77	Joback Method
dvisc	0.0004178	Paxs	473.13	Joback Method
dvisc	0.0002868	Paxs	516.50	Joback Method
dvisc	0.0002087	Paxs	559.86	Joback Method
dvisc	0.0001589	Paxs	603.22	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=R168726&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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