

1-Methyl-2-oxoheptyl acetate

Inchi: InChI=1S/C8H14O3/c1-3-4-5-6-7(9)8(10)11-2/h3-6H2,1-2H3
InchiKey: KKHXXRRGPXSDIJ-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCCCCC(=O)C(=O)OC
Mol. weight [g/mol]: 158.19

Physical Properties

Property code	Value	Unit	Source
gf	-346.36	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.309		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1227.00		NIST Webbook
tb	512.60	K	Joback Method
tc	697.35	K	Joback Method
tf	302.01	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.67	J/molxK	512.60	Joback Method
cpg	310.25	J/molxK	543.39	Joback Method
cpg	321.37	J/molxK	574.18	Joback Method
cpg	332.03	J/molxK	604.98	Joback Method
cpg	342.23	J/molxK	635.77	Joback Method
cpg	351.97	J/molxK	666.56	Joback Method
cpg	361.25	J/molxK	697.35	Joback Method

dvisc	0.0027356	Paxs	302.01	Joback Method
dvisc	0.0015339	Paxs	337.11	Joback Method
dvisc	0.0009592	Paxs	372.21	Joback Method
dvisc	0.0006504	Paxs	407.31	Joback Method
dvisc	0.0004690	Paxs	442.40	Joback Method
dvisc	0.0003549	Paxs	477.50	Joback Method
dvisc	0.0002790	Paxs	512.60	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=R588546&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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