

Methyl 10-oxo-8-decenoate

Inchi:	InChI=1S/C11H18O3/c1-14-11(13)9-7-5-3-2-4-6-8-10-12/h6,8,10H,2-5,7,9H2,1H3/b8-6+
InchiKey:	MRYISIMMTIXZMC-SOFGYWHQSA-N
Formula:	C11H18O3
SMILES:	COC(=O)CCCCCCC=CC=O
Mol. weight [g/mol]:	198.26
CAS:	65114-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-211.48	kJ/mol	Joback Method
hf	-483.53	kJ/mol	Joback Method
hfus	29.52	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.255		Crippen Method
mcvol	170.560	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1592.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2190.00		NIST Webbook
tb	580.19	K	Joback Method
tc	762.53	K	Joback Method
tf	322.81	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.52	J/mol×K	580.19	Joback Method
cpg	432.84	J/mol×K	610.58	Joback Method
cpg	445.55	J/mol×K	640.97	Joback Method
cpg	457.65	J/mol×K	671.36	Joback Method
cpg	469.16	J/mol×K	701.75	Joback Method
cpg	480.11	J/mol×K	732.14	Joback Method

cpg	490.49	J/mol×K	762.53	Joback Method
dvisc	0.0026740	Pa×s	322.81	Joback Method
dvisc	0.0013488	Pa×s	365.71	Joback Method
dvisc	0.0007855	Pa×s	408.60	Joback Method
dvisc	0.0005070	Pa×s	451.50	Joback Method
dvisc	0.0003530	Pa×s	494.40	Joback Method
dvisc	0.0002604	Pa×s	537.29	Joback Method
dvisc	0.0002010	Pa×s	580.19	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=C65114832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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