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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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