

methyl 9-decenoate

Inchi:	InChI=1S/C11H20O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3H,1,4-10H2,2H3
InchiKey:	SBIGSHCJXYGFMX-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	C=CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	184.28

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-389.74	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mvol	168.990	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1316.00		NIST Webbook
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tb	524.05	K	Joback Method
tc	698.08	K	Joback Method
tf	284.13	K	Joback Method
vc	0.656	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.19	J/molxK	524.05	Joback Method
cpg	410.62	J/molxK	553.05	Joback Method
cpg	424.47	J/molxK	582.06	Joback Method
cpg	437.74	J/molxK	611.06	Joback Method
cpg	450.46	J/molxK	640.07	Joback Method
cpg	462.62	J/molxK	669.07	Joback Method
cpg	474.25	J/molxK	698.08	Joback Method
dvisc	0.0029982	Paxs	284.13	Joback Method

dvisc	0.0014650	Paxs	324.12	Joback Method
dvisc	0.0008378	Paxs	364.10	Joback Method
dvisc	0.0005351	Paxs	404.09	Joback Method
dvisc	0.0003706	Paxs	444.08	Joback Method
dvisc	0.0002727	Paxs	484.06	Joback Method
dvisc	0.0002102	Paxs	524.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R283068&Units=SI
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

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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