methyl 9-methyldecanoate

Other names: Methyl isoundecanoate (i-11:0)
Inchi: InChI=1S/C12H24O2/c1-11(2)9-7-5-4-6-8-10-12(13)14-3/h11H,4-10H2,1-3H3
InchiKey: XUSHLLPSFVAOHS-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: COC(=O)CCCCCCCC(C)C
Mol. weight [g/mol]: 200.32
CAS: 5129-55-5

Physical Properties

Property code	Value	Unit	Source
af	0.6457		Cheméo Relay (1.0)
gf	-186.20	kJ/mol	Joback Method
hf	-612.17	kJ/mol	Cheméo Relay (1.0)
hfus	26.10	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-4.23		Cheméo Relay (1.0)
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
tb	501.16	K	Cheméo Relay (1.0)
tc	681.42	K	Cheméo Relay (1.0)
tf	249.61	K	Cheméo Relay (1.0)
vc	0.706	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/mol×K	549.81	Joback Method
cpg	480.46	J/mol×K	578.62	Joback Method
cpg	495.83	J/mol×K	607.44	Joback Method
cpg	510.57	J/mol×K	636.25	Joback Method
cpg	524.69	J/mol×K	665.07	Joback Method
cpg	538.20	J/mol×K	693.88	Joback Method

cpg	551.11	J/mol×K	722.69	Joback Method
dvisc	0.0042661	Pa×s	282.16	Joback Method
dvisc	0.0017460	Pa×s	326.77	Joback Method
dvisc	0.0008857	Pa×s	371.38	Joback Method
dvisc	0.0005197	Pa×s	415.99	Joback Method
dvisc	0.0003381	Pa×s	460.59	Joback Method
dvisc	0.0002373	Pa×s	505.20	Joback Method
dvisc	0.0001764	Pa×s	549.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129555&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume