4-Methyl-undecanal

Inchi: InChI=1S/C12H22O/c1-3-4-5-6-7-9-12(2)10-8-11-13/h8,10-12H,3-7,9H2,1-2H3/b10-8+
InchiKey: WNTNIUKAZPPRFM-CSKARUKUSA-N
Formula: C12H22O
SMILES: CCCCCCCC(C)C=CC=O
Mol. weight [g/mol]: 182.30

Physical Properties

Property code	Value	Unit	Source
gf	28.42	kJ/mol	Joback Method
hf	-264.65	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.738		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
ripol	1630.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	526.34	K	Joback Method
tc	702.92	K	Joback Method
tf	246.92	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.08	J/mol×K	526.34	Joback Method
cpg	434.74	J/mol×K	555.77	Joback Method
cpg	449.67	J/mol×K	585.20	Joback Method
cpg	463.92	J/mol×K	614.63	Joback Method
cpg	477.50	J/mol×K	644.06	Joback Method
cpg	490.44	J/mol×K	673.49	Joback Method
cpg	502.78	J/mol×K	702.92	Joback Method
dvisc	0.0069575	Pa×s	246.92	Joback Method

dvisc	0.0024143	Pa×s	293.49	Joback Method
dvisc	0.0011195	Pa×s	340.06	Joback Method
dvisc	0.0006247	Pa×s	386.63	Joback Method
dvisc	0.0003951	Pa×s	433.20	Joback Method
dvisc	0.0002732	Pa×s	479.77	Joback Method
dvisc	0.0002016	Pa×s	526.34	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=R434652&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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