2-Methyl-decanal

Other names: 2-methyldecan-1-al
Inchi: InChI=1S/C11H22O/c1-3-4-5-6-7-8-9-11(2)10-12/h10-11H,3-9H2,1-2H3
InchiKey: LBICMZLDYMBIGA-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCCCCCCCC(C)C=O
Mol. weight [g/mol]: 170.29
CAS: 19009-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-60.22	kJ/mol	Joback Method
hf	-361.23	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	46.41	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.572		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	499.30	K	Joback Method
tc	670.07	K	Joback Method
tf	240.73	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.78	J/mol×K	499.30	Joback Method
cpg	404.03	J/mol×K	527.76	Joback Method
cpg	418.65	J/mol×K	556.22	Joback Method
cpg	432.66	J/mol×K	584.69	Joback Method

cpg	446.08	J/mol×K	613.15	Joback Method
cpg	458.93	J/mol×K	641.61	Joback Method
cpg	471.22	J/mol×K	670.07	Joback Method
dvisc	0.0076580	Pa×s	240.73	Joback Method
dvisc	0.0028329	Pa×s	283.83	Joback Method
dvisc	0.0013621	Pa×s	326.92	Joback Method
dvisc	0.0007767	Pa×s	370.01	Joback Method
dvisc	0.0004980	Pa×s	413.11	Joback Method
dvisc	0.0003473	Pa×s	456.21	Joback Method
dvisc	0.0002577	Pa×s	499.30	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=C19009564&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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