8-Methyl-6-nonenoic acid

Inchi: InChI=1S/C10H18O2/c1-9(2)7-5-3-4-6-8-10(11)12/h5,7,9H,3-4,6,8H2,1-2H3,(H,11,12)/b7
InchiKey: OCALSPDXYQHUHA-FNORWQNLSA-N
Formula: C10H18O2
SMILES: CC(C)C=CCCCCC(=O)O
Mol. weight [g/mol]: 170.25
CAS: 21382-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-154.64	kJ/mol	Joback Method
hf	-402.60	kJ/mol	Joback Method
hfus	24.02	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.844		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1372.80		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2259.00		NIST Webbook
tb	577.97	K	Joback Method
tc	754.09	K	Joback Method
tf	293.13	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.58	J/mol×K	577.97	Joback Method
cpg	395.79	J/mol×K	607.32	Joback Method
cpg	407.43	J/mol×K	636.68	Joback Method
cpg	418.50	J/mol×K	666.03	Joback Method
cpg	429.05	J/mol×K	695.38	Joback Method
cpg	439.09	J/mol×K	724.73	Joback Method

cpg	448.64	J/mol×K	754.09	Joback Method
dvisc	0.0187361	Pa×s	293.13	Joback Method
dvisc	0.0040298	Pa×s	340.60	Joback Method
dvisc	0.0012624	Pa×s	388.08	Joback Method
dvisc	0.0005093	Pa×s	435.55	Joback Method
dvisc	0.0002456	Pa×s	483.02	Joback Method
dvisc	0.0001350	Pa×s	530.50	Joback Method
dvisc	0.0000818	Pa×s	577.97	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=C21382252&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
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