3-Decenoic acid, (E)-

Other names: E-3-Decenoic acid
Inchi: InChI=1S/C10H18O2/c1-2-3-4-5-6-7-8-9-10(11)12/h7-8H,2-6,9H2,1H3,(H,11,12)/b8-7+
InchiKey: CPVUNKGURQKKKX-BQYQJAHWSA-N
Formula: C10H18O2
SMILES: CCCCCCC=CCC(=O)O
Mol. weight [g/mol]: 170.25
CAS: 53678-20-9

Physical Properties

Property code	Value	Unit	Source
gf	-152.20	kJ/mol	Joback Method
hf	-397.32	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.988		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1366.00		NIST Webbook
ripol	2395.00		NIST Webbook
tb	578.41	K	Joback Method
tc	751.50	K	Joback Method
tf	308.13	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.20	J/mol×K	578.41	Joback Method
cpg	437.66	J/mol×K	722.65	Joback Method
cpg	427.78	J/mol×K	693.80	Joback Method
cpg	417.42	J/mol×K	664.96	Joback Method
cpg	406.55	J/mol×K	636.11	Joback Method
cpg	395.15	J/mol×K	607.26	Joback Method

cpg	447.07	J/mol×K	751.50	Joback Method
dvisc	0.0000873	Pa×s	578.41	Joback Method
dvisc	0.0001391	Pa×s	533.36	Joback Method
dvisc	0.0002417	Pa×s	488.32	Joback Method
dvisc	0.0004699	Pa×s	443.27	Joback Method
dvisc	0.0010616	Pa×s	398.22	Joback Method
dvisc	0.0029530	Pa×s	353.18	Joback Method
dvisc	0.0110783	Pa×s	308.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53678209&Units=SI
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

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

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