

2-Nonynoic acid

Inchi: InChI=1S/C9H14O2/c1-2-3-4-5-6-7-8-9(10)11/h2-6H2,1H3,(H,10,11)
InchiKey: ZAWLBSATNLQTON-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCCCC#CC(=O)O
Mol. weight [g/mol]: 154.21
CAS: 1846-70-4

Physical Properties

Property code	Value	Unit	Source
chl	-5159.30	kJ/mol	NIST Webbook
gf	-38.04	kJ/mol	Joback Method
hf	-221.60	kJ/mol	Joback Method
hfl	-383.10 ± 5.00	kJ/mol	NIST Webbook
hfl	428.40	kJ/mol	NIST Webbook
hfus	27.87	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.045		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	560.37	K	Joback Method
tc	746.82	K	Joback Method
tf	265.15 ± 2.00	K	NIST Webbook
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.89	J/mol×K	560.37	Joback Method
cpg	328.66	J/mol×K	591.44	Joback Method
cpg	338.94	J/mol×K	622.52	Joback Method
cpg	348.75	J/mol×K	653.59	Joback Method
cpg	358.10	J/mol×K	684.67	Joback Method
cpg	367.00	J/mol×K	715.74	Joback Method

cpg	375.48	J/mol×K	746.82	Joback Method
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57127e+01
Coeff. B	-5.02201e+03
Coeff. C	-9.27850e+01
Temperature range (K), min.	418.15
Temperature range (K), max.	575.15

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=C1846704&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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