2-Nonene

Inchi: InChI=1S/C9H18/c1-3-5-7-9-8-6-4-2/h3,5H,4,6-9H2,1-2H3
InchiKey: IICQZTQZQSBHBY-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC=CCCCCCC
Mol. weight [g/mol]: 126.24
CAS: 2216-38-8

Physical Properties

Property code	Value	Unit	Source
gf	105.12	kJ/mol	Joback Method
hf	-111.87	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	35.59	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	909.00		NIST Webbook
tb	421.70 ± 2.00	K	NIST Webbook
tb	423.03 ± 0.40	K	NIST Webbook
tb	422.50 ± 1.50	K	NIST Webbook
tc	580.62	K	Joback Method
tf	181.00 ± 2.00	K	NIST Webbook
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.08	J/mol×K	409.48	Joback Method
cpg	322.32	J/mol×K	552.09	Joback Method
cpg	310.57	J/mol×K	523.57	Joback Method
cpg	298.29	J/mol×K	495.05	Joback Method
cpg	285.46	J/mol×K	466.53	Joback Method

cpg	272.06	J/mol×K	438.00	Joback Method
cpg	333.56	J/mol×K	580.62	Joback Method
dvisc	0.0002012	Pa×s	409.48	Joback Method
dvisc	0.0002654	Pa×s	372.25	Joback Method
dvisc	0.0003724	Pa×s	335.02	Joback Method
dvisc	0.0005686	Pa×s	297.80	Joback Method
dvisc	0.0009797	Pa×s	260.57	Joback Method
dvisc	0.0020238	Pa×s	223.34	Joback Method
dvisc	0.0055889	Pa×s	186.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67432e+01
Coeff. B	-4.37630e+03
Coeff. C	-6.20940e+01
Temperature range (K), min.	328.04
Temperature range (K), max.	444.91

Sources

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=C2216388&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor 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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