1-Chloro-4-nonyne

Inchi: InChI=1S/C9H15Cl/c1-2-3-4-5-6-7-8-9-10/h2-4,7-9H2,1H3
InchiKey: RHZYERSKMQJUCP-UHFFFAOYSA-N
Formula: C9H15Cl
SMILES: CCCCC#CCCCCl
Mol. weight [g/mol]: 158.67
CAS: 3416-74-8

Physical Properties

Property code	Value	Unit	Source
gf	215.77	kJ/mol	Joback Method
hf	27.47	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.199		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	451.75	K	Joback Method
tc	644.56	K	Joback Method
tf	327.21	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.84	J/mol×K	451.75	Joback Method
cpg	288.77	J/mol×K	483.88	Joback Method
cpg	301.13	J/mol×K	516.02	Joback Method
cpg	312.95	J/mol×K	548.15	Joback Method
cpg	324.24	J/mol×K	580.29	Joback Method
cpg	335.01	J/mol×K	612.42	Joback Method
cpg	345.29	J/mol×K	644.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.00	K	5.30	NIST Webbook

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=C3416748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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