3-Hexyne, 2-chloro

Inchi: InChI=1S/C6H9Cl/c1-3-4-5-6(2)7/h6H,3H2,1-2H3
InchiKey: HADUPHFLEHBFLA-UHFFFAOYSA-N
Formula: C6H9Cl
SMILES: CCC#CC(C)Cl
Mol. weight [g/mol]: 116.59

Physical Properties

Property code	Value	Unit	Source
gf	188.07	kJ/mol	Joback Method
hf	84.11	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.027		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	382.67	K	Joback Method
tc	585.85	K	Joback Method
tf	278.40	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.73	J/mol×K	382.67	Joback Method
cpg	170.95	J/mol×K	416.53	Joback Method
cpg	179.78	J/mol×K	450.40	Joback Method
cpg	188.22	J/mol×K	484.26	Joback Method
cpg	196.28	J/mol×K	518.12	Joback Method
cpg	203.98	J/mol×K	551.99	Joback Method
cpg	211.32	J/mol×K	585.85	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=R511234&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume