3-Chloropropylcyclohexane

Other names: Cyclohexane, (3-chloropropyl)-
3-Chloropropylcyclohexane
Inchi: InChI=1S/C9H17Cl/c10-8-4-7-9-5-2-1-3-6-9/h9H,1-8H2
InchiKey: QEISABAAOUXQNG-UHFFFAOYSA-N
Formula: C9H17Cl
SMILES: ClCCCC1CCCCC1
Mol. weight [g/mol]: 160.69

Physical Properties

Property code	Value	Unit	Source
af	0.3495		Cheméo Relay (1.0)
gf	37.42	kJ/mol	Joback Method
hf	-212.28	kJ/mol	Cheméo Relay (1.0)
hfus	15.10	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	Cheméo Relay (1.0)
log10ws	-4.62		Cheméo Relay (1.0)
logp	3.586		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1187.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	481.80	K	Cheméo Relay (1.0)
tc	699.30	K	Cheméo Relay (1.0)
tf	211.41	K	Cheméo Relay (1.0)
vc	0.480	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.70	J/mol×K	462.30	Joback Method
cpg	382.79	J/mol×K	667.94	Joback Method
cpg	369.25	J/mol×K	633.67	Joback Method
cpg	354.89	J/mol×K	599.39	Joback Method

cpg	339.69	J/mol×K	565.12	Joback Method
cpg	323.60	J/mol×K	530.85	Joback Method
cpg	306.62	J/mol×K	496.57	Joback Method
dvisc	0.0008550	Pa×s	345.39	Joback Method
dvisc	0.0002950	Pa×s	462.30	Joback Method
dvisc	0.0003940	Pa×s	423.33	Joback Method
dvisc	0.0005581	Pa×s	384.36	Joback Method
dvisc	0.0073626	Pa×s	228.49	Joback Method
dvisc	0.0014601	Pa×s	306.43	Joback Method
dvisc	0.0029142	Pa×s	267.46	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124625&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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