

3-Cyclohexyl-1-chloropropane

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:	C1CCCC1CCCC1
Mol. weight [g/mol]:	160.68
CAS:	1124-62-5

Physical Properties

Property code	Value	Unit	Source
gf	37.42	kJ/mol	Joback Method
hf	-190.51	kJ/mol	Joback Method
hfus	15.10	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.586		Crippen Method
mvol	139.050	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1187.00		NIST Webbook
tb	462.30	K	Joback Method
tc	667.94	K	Joback Method
tf	228.49	K	Joback Method
vc	0.521	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.70	J/mol×K	462.30	Joback Method
cpg	306.62	J/mol×K	496.57	Joback Method
cpg	323.60	J/mol×K	530.85	Joback Method
cpg	339.69	J/mol×K	565.12	Joback Method
cpg	354.89	J/mol×K	599.39	Joback Method

cpg	369.25	J/molxK	633.67	Joback Method
cpg	382.79	J/molxK	667.94	Joback Method
dvisc	0.0073626	Paxs	228.49	Joback Method
dvisc	0.0029142	Paxs	267.46	Joback Method
dvisc	0.0014601	Paxs	306.43	Joback Method
dvisc	0.0008550	Paxs	345.39	Joback Method
dvisc	0.0005581	Paxs	384.36	Joback Method
dvisc	0.0003940	Paxs	423.33	Joback Method
dvisc	0.0002950	Paxs	462.30	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=C1124625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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