

Chlorocycloheptane

Other names:	Cycloheptane, chloro- Cycloheptyl chloride
Inchi:	InChI=1S/C7H13Cl/c8-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey:	KMJSGLZXFNSANB-UHFFFAOYSA-N
Formula:	C7H13Cl
SMILES:	C1C1CCCCC1
Mol. weight [g/mol]:	132.63
CAS:	2453-46-5

Physical Properties

Property code	Value	Unit	Source
gf	8.48	kJ/mol	Joback Method
hf	-155.39	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	36.16	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.948		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1069.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	420.81	K	Joback Method
tc	640.54	K	Joback Method
tf	202.43	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.90	J/mol×K	420.81	Joback Method
cpg	218.80	J/mol×K	457.43	Joback Method
cpg	234.82	J/mol×K	494.05	Joback Method
cpg	249.97	J/mol×K	530.67	Joback Method

cpg	264.28	J/mol×K	567.29	Joback Method
cpg	277.76	J/mol×K	603.91	Joback Method
cpg	290.44	J/mol×K	640.54	Joback Method
dvisc	0.0127586	Paxs	202.43	Joback Method
dvisc	0.0041917	Paxs	238.83	Joback Method
dvisc	0.0018486	Paxs	275.22	Joback Method
dvisc	0.0009871	Paxs	311.62	Joback Method
dvisc	0.0006010	Paxs	348.02	Joback Method
dvisc	0.0004019	Paxs	384.41	Joback Method
dvisc	0.0002882	Paxs	420.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2453465&Units=SI

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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