

3,4-dichlorohexane (erythro)

Inchi:	InChI=1S/C6H12Cl2/c1-3-5(7)6(8)4-2/h5-6H,3-4H2,1-2H3/t5-,6+
InchiKey:	GBIMAWDSABONCC-OLQVQODUSA-N
Formula:	C6H12Cl2
SMILES:	CCC(Cl)C(Cl)CC
Mol. weight [g/mol]:	155.06

Physical Properties

Property code	Value	Unit	Source
gf	-29.10	kJ/mol	Joback Method
hf	-209.21	kJ/mol	Joback Method
hfus	12.64	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	3.021		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	971.00		NIST Webbook
rinpol	971.00		NIST Webbook
ripol	1218.00		NIST Webbook
tb	410.66	K	Joback Method
tc	599.28	K	Joback Method
tf	187.22	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.29	J/molxK	410.66	Joback Method
cpg	223.08	J/molxK	442.10	Joback Method
cpg	233.37	J/molxK	473.53	Joback Method
cpg	243.19	J/molxK	504.97	Joback Method
cpg	252.55	J/molxK	536.41	Joback Method
cpg	261.47	J/molxK	567.84	Joback Method
cpg	269.95	J/molxK	599.28	Joback Method

dvisc	0.0130601	Paxs	187.22	Joback Method
dvisc	0.0041501	Paxs	224.46	Joback Method
dvisc	0.0018276	Paxs	261.70	Joback Method
dvisc	0.0009873	Paxs	298.94	Joback Method
dvisc	0.0006113	Paxs	336.18	Joback Method
dvisc	0.0004165	Paxs	373.42	Joback Method
dvisc	0.0003042	Paxs	410.66	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=R150715&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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