Cyclohexene, 3-trichloromethyl

Inchi: InChI=1S/C7H9Cl3/c8-7(9,10)6-4-2-1-3-5-6/h2,4,6H,1,3,5H2
InchiKey: DMVOVEXDYGSKIE-UHFFFAOYSA-N
Formula: C7H9Cl3
SMILES: ClC(Cl)(Cl)C1C=CCCC1
Mol. weight [g/mol]: 199.50

Physical Properties

Property code	Value	Unit	Source
gf	29.52	kJ/mol	Joback Method
hf	-131.68	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.713		Crippen Method
mcvol	131.050	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	487.33	K	Joback Method
tc	729.49	K	Joback Method
tf	268.97	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.34	J/mol×K	487.33	Joback Method
cpg	261.70	J/mol×K	527.69	Joback Method
cpg	274.87	J/mol×K	568.05	Joback Method
cpg	286.92	J/mol×K	608.41	Joback Method
cpg	297.92	J/mol×K	648.77	Joback Method
cpg	307.95	J/mol×K	689.13	Joback Method
cpg	317.09	J/mol×K	729.49	Joback Method

dvisc	0.0062681	Pa×s	268.97	Joback Method
dvisc	0.0028832	Pa×s	305.36	Joback Method
dvisc	0.0015648	Pa×s	341.76	Joback Method
dvisc	0.0009552	Pa×s	378.15	Joback Method
dvisc	0.0006359	Pa×s	414.54	Joback Method
dvisc	0.0004521	Pa×s	450.94	Joback Method
dvisc	0.0003382	Pa×s	487.33	Joback Method

Sources

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=R514946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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