2-chloro-2,3,3-trimethylbutane

Inchi: InChI=1S/C7H15Cl/c1-6(2,3)7(4,5)8/h1-5H3
InchiKey: IFMWWVGVDOTBNN-UHFFFAOYSA-N
Formula: C7H15Cl
SMILES: CC(C)(C)C(C)(C)Cl
Mol. weight [g/mol]: 134.65
CAS: 918-07-0

Physical Properties

Property code	Value	Unit	Source
gf	1.81	kJ/mol	Joback Method
hf	-221.05	kJ/mol	Joback Method
hfl	-290.00 ± 3.00	kJ/mol	NIST Webbook
hfus	3.25	kJ/mol	Joback Method
hvap	32.97	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	3.050		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	390.53	K	Joback Method
tc	586.22	K	Joback Method
tf	203.41	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.04	J/mol×K	390.53	Joback Method
cpg	291.01	J/mol×K	553.60	Joback Method
cpg	279.69	J/mol×K	520.99	Joback Method
cpg	267.57	J/mol×K	488.37	Joback Method
cpg	254.62	J/mol×K	455.76	Joback Method
cpg	240.80	J/mol×K	423.14	Joback Method
cpg	301.60	J/mol×K	586.22	Joback Method
dvisc	0.0003558	Pa×s	390.53	Joback Method

dvisc	0.0005102	Pa×s	359.34	Joback Method
dvisc	0.0007835	Pa×s	328.16	Joback Method
dvisc	0.0013167	Pa×s	296.97	Joback Method
dvisc	0.0024993	Pa×s	265.78	Joback Method
dvisc	0.0056252	Pa×s	234.60	Joback Method
dvisc	0.0162368	Pa×s	203.41	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=C918070&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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume