2-chloro-2,3,3-trimethylpentane

Inchi: InChI=1S/C8H17Cl/c1-6-7(2,3)8(4,5)9/h6H2,1-5H3
InchiKey: LKNHZRZTEOZKEA-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCC(C)(C)C(C)(C)Cl
Mol. weight [g/mol]: 148.67
CAS: 69078-89-3

Physical Properties

Property code	Value	Unit	Source
gf	10.23	kJ/mol	Joback Method
hf	-241.69	kJ/mol	Joback Method
hfus	5.84	kJ/mol	Joback Method
hvap	35.20	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	413.41	K	Joback Method
tc	607.51	K	Joback Method
tf	283.75 ± 0.20	K	NIST Webbook
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.40	J/mol×K	413.41	Joback Method
cpg	282.16	J/mol×K	445.76	Joback Method
cpg	296.97	J/mol×K	478.11	Joback Method
cpg	310.86	J/mol×K	510.46	Joback Method
cpg	323.88	J/mol×K	542.81	Joback Method
cpg	336.09	J/mol×K	575.16	Joback Method
cpg	347.54	J/mol×K	607.51	Joback Method
dvisc	0.0149900	Pa×s	214.68	Joback Method
dvisc	0.0051495	Pa×s	247.80	Joback Method

dvisc	0.0022759	Pa×s	280.92	Joback Method
dvisc	0.0011949	Pa×s	314.04	Joback Method
dvisc	0.0007095	Pa×s	347.17	Joback Method
dvisc	0.0004613	Pa×s	380.29	Joback Method
dvisc	0.0003213	Pa×s	413.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1646.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69078893&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume