

1,2,3-trichloro-2-methylbutane

Inchi:	InChI=1S/C5H9Cl3/c1-4(7)5(2,8)3-6/h4H,3H2,1-2H3
InchiKey:	COVUHNHVZQTXPD-UHNVWZDZSA-N
Formula:	C5H9Cl3
SMILES:	CC(Cl)C(C)(Cl)CCl
Mol. weight [g/mol]:	175.48
CAS:	62521-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-44.17	kJ/mol	Joback Method
hf	-207.78	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	38.20	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.850		Crippen Method
mcvol	118.030	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	422.42	K	Joback Method
tc	628.79	K	Joback Method
tf	223.29	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.00	J/molxK	422.42	Joback Method
cpg	211.98	J/molxK	456.82	Joback Method
cpg	221.29	J/molxK	491.21	Joback Method
cpg	229.97	J/molxK	525.61	Joback Method
cpg	238.04	J/molxK	560.00	Joback Method
cpg	245.55	J/molxK	594.40	Joback Method
cpg	252.54	J/molxK	628.79	Joback Method
dvisc	0.0103343	Paxs	223.29	Joback Method
dvisc	0.0041519	Paxs	256.48	Joback Method

dvisc	0.0020557	Paxs	289.67	Joback Method
dvisc	0.0011761	Paxs	322.86	Joback Method
dvisc	0.0007467	Paxs	356.04	Joback Method
dvisc	0.0005122	Paxs	389.23	Joback Method
dvisc	0.0003729	Paxs	422.42	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1616
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62521691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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

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