

1,2,3-Trichlorobutane

Inchi:	InChI=1S/C4H7Cl3/c1-3(6)4(7)2-5/h3-4H,2H2,1H3
InchiKey:	RMZZAEDPBSKZOM-UHFFFAOYSA-N
Formula:	C4H7Cl3
SMILES:	CC(Cl)C(Cl)CCl
Mol. weight [g/mol]:	161.46
CAS:	18338-40-4

Physical Properties

Property code	Value	Unit	Source
gf	-57.87	kJ/mol	Joback Method
hf	-183.67	kJ/mol	Joback Method
hfus	11.66	kJ/mol	Joback Method
hvap	36.88	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.460		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	439.15 ± 1.50	K	NIST Webbook
tc	601.91	K	Joback Method
tf	194.60	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.69	J/mol×K	402.33	Joback Method
cpg	171.34	J/mol×K	435.59	Joback Method
cpg	178.58	J/mol×K	468.86	Joback Method
cpg	185.45	J/mol×K	502.12	Joback Method
cpg	191.94	J/mol×K	535.38	Joback Method
cpg	198.08	J/mol×K	568.64	Joback Method
cpg	203.87	J/mol×K	601.91	Joback Method
dvisc	0.0106392	Pa×s	194.60	Joback Method
dvisc	0.0039497	Pa×s	229.22	Joback Method

dvisc	0.0019018	Pa×s	263.84	Joback Method
dvisc	0.0010849	Pa×s	298.47	Joback Method
dvisc	0.0006955	Pa×s	333.09	Joback Method
dvisc	0.0004848	Pa×s	367.71	Joback Method
dvisc	0.0003596	Pa×s	402.33	Joback Method
hvapt	41.30	kJ/mol	357.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C18338404&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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