trichlorotoluene

Other names: Benzene, trichloromethyl-
Inchi: InChI=1S/C7H5Cl3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H
InchiKey: XEMRAKSQROQPBR-UHFFFAOYSA-N
Formula: C7H5Cl3
SMILES: ClC(Cl)(Cl)c1ccccc1
Mol. weight [g/mol]: 195.47
CAS: 30583-33-6

Physical Properties

Property code	Value	Unit	Source
chl	-3494.90 ± 1.80	kJ/mol	NIST Webbook
gf	87.52	kJ/mol	Joback Method
hf	12.50 ± 2.30	kJ/mol	NIST Webbook
hfl	-45.10 ± 2.00	kJ/mol	NIST Webbook
hfus	13.10	kJ/mol	Joback Method
hvap	57.60 ± 1.20	kJ/mol	NIST Webbook
log10ws	-3.47		Crippen Method
logp	3.513		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	495.30	K	Joback Method
tc	744.27	K	Joback Method
tf	287.25	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.89	J/mol×K	495.30	Joback Method
cpg	223.35	J/mol×K	536.79	Joback Method
cpg	232.76	J/mol×K	578.29	Joback Method
cpg	241.20	J/mol×K	619.78	Joback Method
cpg	248.77	J/mol×K	661.28	Joback Method
cpg	255.53	J/mol×K	702.77	Joback Method

cpg	261.58	J/mol×K	744.27	Joback Method
dvisc	0.0039216	Pa×s	287.25	Joback Method
dvisc	0.0020289	Pa×s	321.93	Joback Method
dvisc	0.0011932	Pa×s	356.60	Joback Method
dvisc	0.0007709	Pa×s	391.27	Joback Method
dvisc	0.0005348	Pa×s	425.95	Joback Method
dvisc	0.0003920	Pa×s	460.62	Joback Method
dvisc	0.0003001	Pa×s	495.30	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C30583336&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
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