

chlorotoluene

Other names:	Benzyl chloride
Inchi:	InChI=1S/C7H7Cl/c1-6-4-2-3-5-7(6)8/h2-5H,1H3
InchiKey:	IBSQPLPBRSHTTG-UHFFFAOYSA-N
Formula:	C7H7Cl
SMILES:	Cc1cccc1Cl
Mol. weight [g/mol]:	126.58
CAS:	25168-05-2

Physical Properties

Property code	Value	Unit	Source
gf	98.91	kJ/mol	Joback Method
hf	21.51	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	38.50	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.648		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	962.00		NIST Webbook
tb	428.65	K	Joback Method
tc	649.87	K	Joback Method
tf	237.51	K	Joback Method
vc	0.368	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.77	J/mol×K	428.65	Joback Method
cpg	174.12	J/mol×K	465.52	Joback Method
cpg	183.86	J/mol×K	502.39	Joback Method
cpg	193.00	J/mol×K	539.26	Joback Method
cpg	201.57	J/mol×K	576.13	Joback Method
cpg	209.60	J/mol×K	613.00	Joback Method
cpg	217.11	J/mol×K	649.87	Joback Method

dvisc	0.0021341	Paxs	237.51	Joback Method
dvisc	0.0012200	Paxs	269.37	Joback Method
dvisc	0.0007850	Paxs	301.22	Joback Method
dvisc	0.0005496	Paxs	333.08	Joback Method
dvisc	0.0004094	Paxs	364.94	Joback Method
dvisc	0.0003198	Paxs	396.79	Joback Method
dvisc	0.0002591	Paxs	428.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25168052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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