

m-Tert-butyl chlorobenzene

Inchi:	InChI=1S/C10H13Cl/c1-10(2,3)8-5-4-6-9(11)7-8/h4-7H,1-3H3
InchiKey:	KYXNATZCTBFSTH-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CC(C)(C)c1cccc(Cl)c1
Mol. weight [g/mol]:	168.66
CAS:	3972-55-2

Physical Properties

Property code	Value	Unit	Source
gf	127.01	kJ/mol	Joback Method
hf	-49.16	kJ/mol	Joback Method
hfl	-109.00 ± 0.80	kJ/mol	NIST Webbook
hfus	12.09	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.637		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	494.06	K	Joback Method
tc	720.15	K	Joback Method
tf	273.74	K	Joback Method
vc	0.525	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.69	J/molxK	494.06	Joback Method
cpg	303.90	J/molxK	531.74	Joback Method
cpg	318.04	J/molxK	569.42	Joback Method
cpg	331.18	J/molxK	607.10	Joback Method
cpg	343.37	J/molxK	644.79	Joback Method
cpg	354.69	J/molxK	682.47	Joback Method
cpg	365.18	J/molxK	720.15	Joback Method
dvisc	0.0033165	Paxs	273.74	Joback Method

dvisc	0.0016285	Paxs	310.46	Joback Method
dvisc	0.0009295	Paxs	347.18	Joback Method
dvisc	0.0005906	Paxs	383.90	Joback Method
dvisc	0.0004062	Paxs	420.62	Joback Method
dvisc	0.0002967	Paxs	457.34	Joback Method
dvisc	0.0002270	Paxs	494.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3972552&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

Legend

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

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