

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)c1ccccc(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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.69	J/mol×K	494.06	Joback Method
cpg	354.69	J/mol×K	682.47	Joback Method
cpg	343.37	J/mol×K	644.79	Joback Method
cpg	331.18	J/mol×K	607.10	Joback Method
cpg	318.04	J/mol×K	569.42	Joback Method
cpg	303.90	J/mol×K	531.74	Joback Method
cpg	365.18	J/mol×K	720.15	Joback Method
dvisc	0.0002270	Pa×s	494.06	Joback Method

dvisc	0.0002967	Pa×s	457.34	Joback Method
dvisc	0.0004062	Pa×s	420.62	Joback Method
dvisc	0.0005906	Pa×s	383.90	Joback Method
dvisc	0.0009295	Pa×s	347.18	Joback Method
dvisc	0.0016285	Pa×s	310.46	Joback Method
dvisc	0.0033165	Pa×s	273.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3972552&Units=SI
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

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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