Chloropentamethylbenzene

Inchi: InChI=1S/C11H15Cl/c1-6-7(2)9(4)11(12)10(5)8(6)3/h1-5H3
InchiKey: GWKDRPNLSOEGRT-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: Cc1c(C)c(C)c(Cl)c(C)c1C
Mol. weight [g/mol]: 182.69
CAS: 5153-39-9

Physical Properties

Property code	Value	Unit	Source
gf	94.07	kJ/mol	Joback Method
hf	-106.93	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	50.05	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.882		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
ss	311.48	J/mol×K	NIST Webbook
tb	540.09	K	Joback Method
tc	753.12	K	Joback Method
tf	427.00 ± 2.00	K	NIST Webbook
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.05	J/mol×K	540.09	Joback Method
cpg	402.60	J/mol×K	753.12	Joback Method
cpg	391.96	J/mol×K	717.61	Joback Method
cpg	380.76	J/mol×K	682.11	Joback Method
cpg	368.97	J/mol×K	646.60	Joback Method
cpg	356.60	J/mol×K	611.10	Joback Method
cpg	343.62	J/mol×K	575.59	Joback Method
cps	244.60	J/mol×K	300.00	NIST Webbook

dvisc	0.0001966	Pa×s	540.09	Joback Method
dvisc	0.0002317	Pa×s	505.52	Joback Method
dvisc	0.0002796	Pa×s	470.95	Joback Method
dvisc	0.0003476	Pa×s	436.38	Joback Method
dvisc	0.0004487	Pa×s	401.81	Joback Method
dvisc	0.0006077	Pa×s	367.24	Joback Method
dvisc	0.0008765	Pa×s	332.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5153399&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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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