

1,2,3,4-Tetramethyl-5-(chloromethyl)benzene

Inchi:	InChI=1S/C11H15Cl/c1-7-5-11(6-12)10(4)9(3)8(7)2/h5H,6H2,1-4H3
InchiKey:	IWOZCBWTEAPSSJ-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	Cc1cc(CCl)c(C)c(C)c1C
Mol. weight [g/mol]:	182.69

Physical Properties

Property code	Value	Unit	Source
gf	103.70	kJ/mol	Joback Method
hf	-95.46	kJ/mol	Joback Method
hfus	20.93	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.659		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinsol	1517.00		NIST Webbook
tb	535.11	K	Joback Method
tc	747.03	K	Joback Method
tf	320.15	K	Joback Method
vc	0.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.24	J/molxK	535.11	Joback Method
cpg	344.12	J/molxK	570.43	Joback Method
cpg	357.35	J/molxK	605.75	Joback Method
cpg	369.92	J/molxK	641.07	Joback Method
cpg	381.87	J/molxK	676.39	Joback Method
cpg	393.19	J/molxK	711.71	Joback Method
cpg	403.92	J/molxK	747.03	Joback Method
dvisc	0.0010904	Paxs	320.15	Joback Method
dvisc	0.0007142	Paxs	355.98	Joback Method

dvisc	0.0005055	Paxs	391.80	Joback Method
dvisc	0.0003791	Paxs	427.63	Joback Method
dvisc	0.0002972	Paxs	463.46	Joback Method
dvisc	0.0002413	Paxs	499.28	Joback Method
dvisc	0.0002014	Paxs	535.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
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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