2,3,5,6-Tetramethylbenzyl chloride

Other names:	Benzene, 3-(chloromethyl)-1,2,4,5-tetramethyl-
	3-(Chloromethyl)-1,2,4,5-tetramethylbenzene
Inchi:	InChI=1S/C11H15Cl/c1-7-5-8(2)10(4)11(6-12)9(7)3/h5H,6H2,1-4H3
InchiKey:	UGAPPXGBBWAIGT-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	Cc1cc(C)c(C)c(CCl)c1C
Mol. weight [g/mol]:	182.69
CAS:	7435-83-8

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
rinpol	1478.00		NIST Webbook
tb	535.11	K	Joback Method
tc	747.03	K	Joback Method
tf	320.15	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.24	J/mol×K	535.11	Joback Method
cpg	393.19	J/mol×K	711.71	Joback Method
cpg	381.87	J/mol×K	676.39	Joback Method
cpg	369.92	J/mol×K	641.07	Joback Method
cpg	357.35	J/mol×K	605.75	Joback Method
cpg	344.12	J/mol×K	570.43	Joback Method

cpg	403.92	J/mol×K	747.03	Joback Method
dvisc	0.0002014	Pa×s	535.11	Joback Method
dvisc	0.0002413	Pa×s	499.28	Joback Method
dvisc	0.0002972	Pa×s	463.46	Joback Method
dvisc	0.0003791	Pa×s	427.63	Joback Method
dvisc	0.0005055	Pa×s	391.80	Joback Method
dvisc	0.0007142	Pa×s	355.98	Joback Method
dvisc	0.0010904	Pa×s	320.15	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7435838&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
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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