

Benzene, 1-chloro-2,3,5,6-tetramethyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H13Cl/c1-6-5-7(2)9(4)10(11)8(6)3/h5H,1-4H3

HNXWCWJCZMYBDF-UHFFFAOYSA-N

C10H13Cl

Cc1cc(C)c(C)c(Cl)c1C

168.66

Physical Properties

Property code	Value	Unit	Source
gf	95.28	kJ/mol	Joback Method
hf	-74.82	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.574		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1267.00		NIST Webbook
rinpol	1267.00		NIST Webbook
tb	512.23	K	Joback Method
tc	727.62	K	Joback Method
tf	308.88	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.81	J/mol×K	512.23	Joback Method
cpg	344.14	J/mol×K	691.72	Joback Method
cpg	333.63	J/mol×K	655.83	Joback Method
cpg	322.56	J/mol×K	619.93	Joback Method
cpg	310.90	J/mol×K	584.03	Joback Method
cpg	298.66	J/mol×K	548.13	Joback Method
cpg	354.10	J/mol×K	727.62	Joback Method
dvisc	0.0002113	Pa×s	512.23	Joback Method

dvisc	0.0002512	Pa×s	478.34	Joback Method
dvisc	0.0003067	Pa×s	444.45	Joback Method
dvisc	0.0003870	Pa×s	410.56	Joback Method
dvisc	0.0005091	Pa×s	376.66	Joback Method
dvisc	0.0007072	Pa×s	342.77	Joback Method
dvisc	0.0010557	Pa×s	308.88	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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