Benzene, 3-chloro-1,2,4-trimethyl

Inchi: InChI=1S/C9H11Cl/c1-6-4-5-7(2)9(10)8(6)3/h4-5H,1-3H3
InchiKey: AXJGVZMSADXTDE-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: Cc1ccc(C)c(Cl)c1C
Mol. weight [g/mol]: 154.64

Physical Properties

Property code	Value	Unit	Source
gf	96.49	kJ/mol	Joback Method
hf	-42.71	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.265		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	484.37	K	Joback Method
tc	701.99	K	Joback Method
tf	285.09	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.34	J/mol×K	484.37	Joback Method
cpg	297.78	J/mol×K	665.72	Joback Method
cpg	288.04	J/mol×K	629.45	Joback Method
cpg	277.74	J/mol×K	593.18	Joback Method
cpg	266.86	J/mol×K	556.91	Joback Method
cpg	255.40	J/mol×K	520.64	Joback Method

cpg	306.99	J/mol×K	701.99	Joback Method
dvisc	0.0002266	Pa×s	484.37	Joback Method
dvisc	0.0002723	Pa×s	451.16	Joback Method
dvisc	0.0003370	Pa×s	417.94	Joback Method
dvisc	0.0004325	Pa×s	384.73	Joback Method
dvisc	0.0005820	Pa×s	351.52	Joback Method
dvisc	0.0008333	Pa×s	318.30	Joback Method
dvisc	0.0012970	Pa×s	285.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132084&Units=SI

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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