Benzene, 1-chloromethyl-3,5-dimethyl-4-(1-methylethyl)

Inchi: InChI=1S/C12H17Cl/c1-8(2)12-9(3)5-11(7-13)6-10(12)4/h5-6,8H,7H2,1-4H3

InchiKey: KPOPLJCWVAAYJX-UHFFFAOYSA-N

Formula: C12H17Cl

SMILES: Cc1cc(CCl)cc(C)c1C(C)C

Mol. weight [g/mol]: 196.72

Physical Properties

Property code	Value	Unit	Source
gf	119.31	kJ/mol	Joback Method
hf	-109.91	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	50.56	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.166		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1447.00		NIST Webbook
tb	552.57	K	Joback Method
tc	764.55	K	Joback Method
tf	303.90	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.00	J/mol×K	552.57	Joback Method
cpg	392.45	J/mol×K	587.90	Joback Method
cpg	407.10	J/mol×K	623.23	Joback Method
cpg	420.97	J/mol×K	658.56	Joback Method
cpg	434.08	J/mol×K	693.89	Joback Method
cpg	446.46	J/mol×K	729.22	Joback Method
cpg	458.13	J/mol×K	764.55	Joback Method
dvisc	0.0017529	Pa×s	303.90	Joback Method
dvisc	0.0009583	Pa×s	345.35	Joback Method

dvisc	0.0005963	Pa×s	386.79	Joback Method
dvisc	0.0004067	Pa×s	428.24	Joback Method
dvisc	0.0002968	Pa×s	469.68	Joback Method
dvisc	0.0002279	Pa×s	511.12	Joback Method
dvisc	0.0001821	Pa×s	552.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131843&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