Benzene, 2-(chloromethyl)-1-methyl-4-(1,1-dimethylethyl)

Other names: 1-Methyl-4-(1,1-dimethylethyl)-2-chloromethylbenzene
Inchi: InChI=1S/C12H17Cl/c1-9-5-6-11(12(2,3)4)7-10(9)8-13/h5-7H,8H2,1-4H3
InchiKey: HALFEDSYDFTNIW-UHFFFAOYSA-N
Formula: C12H17Cl
SMILES: Cc1ccc(C(C)(C)C)cc1CCl
Mol. weight [g/mol]: 196.72

Physical Properties

Property code	Value	Unit	Source
gf	134.22	kJ/mol	Joback Method
hf	-101.91	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	49.00	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.031		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1426.00		NIST Webbook
tb	544.80	K	Joback Method
tc	764.31	K	Joback Method
tf	308.80	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.93	J/mol×K	544.80	Joback Method
cpg	452.12	J/mol×K	727.72	Joback Method
cpg	439.55	J/mol×K	691.14	Joback Method
cpg	426.10	J/mol×K	654.55	Joback Method
cpg	411.72	J/mol×K	617.97	Joback Method
cpg	396.35	J/mol×K	581.38	Joback Method
cpg	463.87	J/mol×K	764.31	Joback Method

dvisc	0.0001842	Pa×s	544.80	Joback Method
dvisc	0.0002377	Pa×s	505.47	Joback Method
dvisc	0.0003201	Pa×s	466.13	Joback Method
dvisc	0.0004554	Pa×s	426.80	Joback Method
dvisc	0.0006960	Pa×s	387.47	Joback Method
dvisc	0.0011706	Pa×s	348.13	Joback Method
dvisc	0.0022477	Pa×s	308.80	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=R132059&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