

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

Inchi:	InChI=1S/C12H17Cl/c1-9-7-11(12(2,3)4)6-5-10(9)8-13/h5-7H,8H2,1-4H3
InchiKey:	DDMGSGAOLZOB-UHFFFAOYSA-N
Formula:	C12H17Cl
SMILES:	Cc1cc(C(C)(C)C)ccc1CCl
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
mvol	168.420	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1442.00		NIST Webbook
tb	544.80	K	Joback Method
tc	764.31	K	Joback Method
tf	308.80	K	Joback Method
vc	0.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.93	J/molxK	544.80	Joback Method
cpg	396.35	J/molxK	581.38	Joback Method
cpg	411.72	J/molxK	617.97	Joback Method
cpg	426.10	J/molxK	654.55	Joback Method
cpg	439.55	J/molxK	691.14	Joback Method
cpg	452.12	J/molxK	727.72	Joback Method
cpg	463.87	J/molxK	764.31	Joback Method
dvisc	0.0022477	Paxs	308.80	Joback Method
dvisc	0.0011706	Paxs	348.13	Joback Method

dvisc	0.0006960	Paxs	387.47	Joback Method
dvisc	0.0004554	Paxs	426.80	Joback Method
dvisc	0.0003201	Paxs	466.13	Joback Method
dvisc	0.0002377	Paxs	505.47	Joback Method
dvisc	0.0001842	Paxs	544.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R131823&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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