1-Methyl-4-(1-methylethyl)-2-(chloromethyl)benze

Inchi: InChI=1S/C11H15Cl/c1-8(2)10-5-4-9(3)11(6-10)7-12/h4-6,8H,7H2,1-3H3
InchiKey: LZQCWOMPPBNFOA-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: Cc1ccc(C(C)C)cc1CCl
Mol. weight [g/mol]: 182.69

Physical Properties

Property code	Value	Unit	Source
gf	120.52	kJ/mol	Joback Method
hf	-77.80	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	47.68	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.857		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1346.00		NIST Webbook
tb	524.71	K	Joback Method
tc	739.09	K	Joback Method
tf	280.11	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.60	J/mol×K	524.71	Joback Method
cpg	345.53	J/mol×K	560.44	Joback Method
cpg	359.65	J/mol×K	596.17	Joback Method
cpg	372.97	J/mol×K	631.90	Joback Method
cpg	385.54	J/mol×K	667.63	Joback Method
cpg	397.37	J/mol×K	703.36	Joback Method
cpg	408.49	J/mol×K	739.09	Joback Method
dvisc	0.0023785	Pa×s	280.11	Joback Method
dvisc	0.0012121	Pa×s	320.88	Joback Method

dvisc	0.0007191	Pa×s	361.64	Joback Method
dvisc	0.0004742	Pa×s	402.41	Joback Method
dvisc	0.0003376	Pa×s	443.18	Joback Method
dvisc	0.0002545	Pa×s	483.94	Joback Method
dvisc	0.0002005	Pa×s	524.71	Joback Method

Sources

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=R520406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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