Benzene, 1-chloro-3-(2,2-dimethyl-1-methylenepropyl)-

Inchi: InChI=1S/C12H15Cl/c1-9(12(2,3)4)10-6-5-7-11(13)8-10/h5-8H,1H2,2-4H3
InchiKey: XROWFHHSVOICSU-UHFFFAOYSA-N
Formula: C12H15Cl
SMILES: C=C(c1cccc(Cl)c1)C(C)(C)C
Mol. weight [g/mol]: 194.70
CAS: 146558-43-2

Physical Properties

Property code	Value	Unit	Source
affp	839.80	kJ/mol	NIST Webbook
basg	811.00	kJ/mol	NIST Webbook
gf	223.14	kJ/mol	Joback Method
hf	25.20	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	47.74	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.399		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	536.38	K	Joback Method
tc	763.90	K	Joback Method
tf	280.56	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.41	J/mol×K	536.38	Joback Method
cpg	376.82	J/mol×K	574.30	Joback Method
cpg	392.04	J/mol×K	612.22	Joback Method
cpg	406.17	J/mol×K	650.14	Joback Method
cpg	419.26	J/mol×K	688.06	Joback Method
cpg	431.41	J/mol×K	725.98	Joback Method
cpg	442.68	J/mol×K	763.90	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=C146558432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume