Benzene, 2-chloro-4-(2,2-dimethyl-1-methylenepropyl)-1-me

Inchi: InChI=1S/C13H17ClO/c1-9(13(2,3)4)10-6-7-12(15-5)11(14)8-10/h6-8H,1H2,2-5H3
InchiKey: JMYOLRCCLQTNIL-UHFFFAOYSA-N
Formula: C13H17ClO
SMILES: C=C(c1ccc(OC)c(Cl)c1)C(C)(C)C
Mol. weight [g/mol]: 224.73
CAS: 146558-40-9

Physical Properties

Property code	Value	Unit	Source
affp	883.00	kJ/mol	NIST Webbook
basg	854.20	kJ/mol	NIST Webbook
gf	116.93	kJ/mol	Joback Method
hf	-139.13	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	53.04	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.408		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
tb	586.66	K	Joback Method
tc	808.25	K	Joback Method
tf	326.58	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.42	J/mol×K	586.66	Joback Method
cpg	449.66	J/mol×K	623.59	Joback Method
cpg	464.86	J/mol×K	660.52	Joback Method
cpg	479.08	J/mol×K	697.45	Joback Method
cpg	492.37	J/mol×K	734.38	Joback Method
cpg	504.77	J/mol×K	771.31	Joback Method
cpg	516.33	J/mol×K	808.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146558409&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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