Benzene, chloro, 1,2-dimethyl, 4-(1,1-dimethylethyl)

Inchi: InChI=1S/C12H17Cl/c1-8-6-10(12(3,4)5)7-11(13)9(8)2/h6-7H,1-5H3
InchiKey: FQYVVTUJLJWGJX-UHFFFAOYSA-N
Formula: C12H17Cl
SMILES: Cc1cc(C(C)(C)C)cc(Cl)c1C
Mol. weight [g/mol]: 196.72

Physical Properties

Property code	Value	Unit	Source
gf	124.59	kJ/mol	Joback Method
hf	-113.38	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	49.66	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.254		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
tb	549.78	K	Joback Method
tc	770.39	K	Joback Method
tf	321.32	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.95	J/mol×K	549.78	Joback Method
cpg	450.98	J/mol×K	733.62	Joback Method
cpg	438.55	J/mol×K	696.85	Joback Method
cpg	425.28	J/mol×K	660.09	Joback Method
cpg	411.12	J/mol×K	623.32	Joback Method
cpg	396.03	J/mol×K	586.55	Joback Method

cpg	462.63	J/mol×K	770.39	Joback Method
dvisc	0.0001790	Pa×s	549.78	Joback Method
dvisc	0.0002263	Pa×s	511.70	Joback Method
dvisc	0.0002970	Pa×s	473.63	Joback Method
dvisc	0.0004089	Pa×s	435.55	Joback Method
dvisc	0.0005985	Pa×s	397.47	Joback Method
dvisc	0.0009497	Pa×s	359.40	Joback Method
dvisc	0.0016810	Pa×s	321.32	Joback Method

Sources

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=R131561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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