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	1400.00		NIST Webbook
rinpol	1392.00		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	396.03	J/mol×K	586.55	Joback Method
cpg	411.12	J/mol×K	623.32	Joback Method
cpg	425.28	J/mol×K	660.09	Joback Method
cpg	438.55	J/mol×K	696.85	Joback Method
cpg	450.98	J/mol×K	733.62	Joback Method

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

Sources

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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