

Benzene, 2-(4-chlorobutyl)-1,4-dimethyl

Inchi:	InChI=1S/C12H17Cl/c1-10-6-7-11(2)12(9-10)5-3-4-8-13/h6-7,9H,3-5,8H2,1-2H3
InchiKey:	HREQIFZHXURJBY-UHFFFAOYSA-N
Formula:	C12H17Cl
SMILES:	<chem>Cc1ccc(C)c(CCCCl)c1</chem>
Mol. weight [g/mol]:	196.72

Physical Properties

Property code	Value	Unit	Source
gf	131.38	kJ/mol	Joback Method
hf	-93.16	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.865		Crippen Method
mvol	168.420	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	548.03	K	Joback Method
tc	754.46	K	Joback Method
tf	306.38	K	Joback Method
vc	0.648	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.70	J/molxK	548.03	Joback Method
cpg	392.06	J/molxK	582.44	Joback Method
cpg	406.60	J/molxK	616.84	Joback Method
cpg	420.36	J/molxK	651.25	Joback Method
cpg	433.37	J/molxK	685.65	Joback Method
cpg	445.65	J/molxK	720.06	Joback Method
cpg	457.23	J/molxK	754.46	Joback Method
dvisc	0.0018302	Paxs	306.38	Joback Method

dvisc	0.0010196	Paxs	346.65	Joback Method
dvisc	0.0006416	Paxs	386.93	Joback Method
dvisc	0.0004406	Paxs	427.20	Joback Method
dvisc	0.0003228	Paxs	467.48	Joback Method
dvisc	0.0002485	Paxs	507.75	Joback Method
dvisc	0.0001988	Paxs	548.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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