Benzene, 2-(3-chlorobutyl)-1,4-dimethyl

Inchi: InChI=1S/C12H17Cl/c1-9-4-5-10(2)12(8-9)7-6-11(3)13/h4-5,8,11H,6-7H2,1-3H3
InchiKey: WHGMHBOCPNYHGF-UHFFFAOYSA-N
Formula: C12H17Cl
SMILES: Cc1ccc(C)c(CCC(C)Cl)c1
Mol. weight [g/mol]: 196.72

Physical Properties

Property code	Value	Unit	Source
gf	128.94	kJ/mol	Joback Method
hf	-98.44	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	49.90	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.863		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1446.00		NIST Webbook
tb	547.59	K	Joback Method
tc	758.50	K	Joback Method
tf	291.38	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.01	J/mol×K	547.59	Joback Method
cpg	447.52	J/mol×K	723.34	Joback Method
cpg	435.02	J/mol×K	688.19	Joback Method
cpg	421.74	J/mol×K	653.04	Joback Method
cpg	407.67	J/mol×K	617.89	Joback Method
cpg	392.77	J/mol×K	582.74	Joback Method
cpg	459.29	J/mol×K	758.50	Joback Method
dvisc	0.0001867	Pa×s	547.59	Joback Method
dvisc	0.0002383	Pa×s	504.89	Joback Method

dvisc	0.0003182	Pa×s	462.19	Joback Method
dvisc	0.0004507	Pa×s	419.49	Joback Method
dvisc	0.0006907	Pa×s	376.78	Joback Method
dvisc	0.0011807	Pa×s	334.08	Joback Method
dvisc	0.0023617	Pa×s	291.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131927&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