Benzene, 3-butyl-1(chloromethyl)-4-methyl

Inchi: InChI=1S/C11H15Cl/c1-3-4-11-7-10(8-12)6-5-9(11)2/h5-7H,3-4,8H2,1-2H3
InchiKey: HZVZMQXEFWZFHU-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: CCCc1cc(CCl)ccc1C
Mol. weight [g/mol]: 182.69

Physical Properties

Property code	Value	Unit	Source
gf	122.96	kJ/mol	Joback Method
hf	-72.52	kJ/mol	Joback Method
hfus	21.71	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.686		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	525.15	K	Joback Method
tc	734.82	K	Joback Method
tf	295.11	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.32	J/mol×K	525.15	Joback Method
cpg	344.85	J/mol×K	560.10	Joback Method
cpg	358.61	J/mol×K	595.04	Joback Method
cpg	371.63	J/mol×K	629.99	Joback Method
cpg	383.92	J/mol×K	664.93	Joback Method
cpg	395.52	J/mol×K	699.88	Joback Method
cpg	406.46	J/mol×K	734.82	Joback Method
dvisc	0.0018269	Pa×s	295.11	Joback Method

dvisc	0.0010391	Pa×s	333.45	Joback Method
dvisc	0.0006639	Pa×s	371.79	Joback Method
dvisc	0.0004612	Pa×s	410.13	Joback Method
dvisc	0.0003410	Pa×s	448.47	Joback Method
dvisc	0.0002645	Pa×s	486.81	Joback Method
dvisc	0.0002128	Pa×s	525.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132079&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