3-chloro-2-butoxy-tetrahydro-pyran

Inchi: InChI=1S/C9H17ClO2/c1-2-3-6-11-9-8(10)5-4-7-12-9/h8-9H,2-7H2,1H3
InchiKey: YVJCTCVZSCULEB-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCOC1OCCCC1Cl
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-161.41	kJ/mol	Joback Method
hf	-475.07	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.547		Crippen Method
mcvol	150.790	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
tb	507.00	K	Joback Method
tc	709.81	K	Joback Method
tf	273.05	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.05	J/mol×K	507.00	Joback Method
cpg	365.23	J/mol×K	540.80	Joback Method
cpg	381.62	J/mol×K	574.60	Joback Method
cpg	397.21	J/mol×K	608.40	Joback Method
cpg	412.01	J/mol×K	642.20	Joback Method
cpg	426.03	J/mol×K	676.01	Joback Method
cpg	439.27	J/mol×K	709.81	Joback Method
dvisc	0.0036685	Pa×s	273.05	Joback Method

dvisc	0.0018009	Pa×s	312.04	Joback Method
dvisc	0.0010355	Pa×s	351.03	Joback Method
dvisc	0.0006650	Pa×s	390.02	Joback Method
dvisc	0.0004629	Pa×s	429.02	Joback Method
dvisc	0.0003423	Pa×s	468.01	Joback Method
dvisc	0.0002651	Pa×s	507.00	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132920&Units=SI

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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