

2H-Pyran, tetrahydro, 3-chloro-2-butoxy, # 2

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
mvol	150.790	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	507.00	K	Joback Method
tc	709.81	K	Joback Method
tf	273.05	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0018009	Paxs	312.04	Joback Method
dvisc	0.0010355	Paxs	351.03	Joback Method
dvisc	0.0006650	Paxs	390.02	Joback Method
dvisc	0.0004629	Paxs	429.02	Joback Method
dvisc	0.0003423	Paxs	468.01	Joback Method
dvisc	0.0002651	Paxs	507.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90975&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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