2-propoxy-3-chloro-tetrahydro-furan

Other names: Tetrahydrofuran, 3-chloro-2-propyloxy
Inchi: InChI=1S/C7H13ClO2/c1-2-4-9-7-6(8)3-5-10-7/h6-7H,2-5H2,1H3
InchiKey: ZQKWVRVZQFSFFG-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCCOC1OCCC1Cl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-166.15	kJ/mol	Joback Method
hf	-427.63	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	42.43	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.767		Crippen Method
mcvol	122.610	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
tb	456.97	K	Joback Method
tc	657.57	K	Joback Method
tf	254.03	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.25	J/mol×K	456.97	Joback Method
cpg	273.51	J/mol×K	490.40	Joback Method
cpg	287.15	J/mol×K	523.84	Joback Method
cpg	300.16	J/mol×K	557.27	Joback Method
cpg	312.55	J/mol×K	590.70	Joback Method
cpg	324.33	J/mol×K	624.14	Joback Method

cpg	335.51	J/mol×K	657.57	Joback Method
dvisc	0.0026765	Pa×s	254.03	Joback Method
dvisc	0.0015701	Pa×s	287.85	Joback Method
dvisc	0.0010304	Pa×s	321.68	Joback Method
dvisc	0.0007327	Pa×s	355.50	Joback Method
dvisc	0.0005527	Pa×s	389.32	Joback Method
dvisc	0.0004362	Pa×s	423.15	Joback Method
dvisc	0.0003565	Pa×s	456.97	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=R91329&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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