8-Chloro-1-octanol

Other names: 1-Octanol, 8-chloro-
8-chlorooctan-1-ol
Inchi: InChI=1S/C8H17ClO/c9-7-5-3-1-2-4-6-8-10/h10H,1-8H2
InchiKey: YDFAJMDFCCJZSI-UHFFFAOYSA-N
Formula: C8H17ClO
SMILES: OCCCCCCCCCl
Mol. weight [g/mol]: 164.67
CAS: 23144-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-132.27	kJ/mol	Joback Method
hf	-376.42	kJ/mol	Joback Method
hfus	24.76	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.558		Crippen Method
mcvol	141.690	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1351.70		NIST Webbook
rinpol	1351.70		NIST Webbook
tb	512.05	K	Joback Method
tc	677.36	K	Joback Method
tf	270.66	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.41	J/mol×K	512.05	Joback Method
cpg	329.53	J/mol×K	539.60	Joback Method
cpg	340.21	J/mol×K	567.15	Joback Method
cpg	350.45	J/mol×K	594.71	Joback Method
cpg	360.27	J/mol×K	622.26	Joback Method

cpg	369.68	J/mol×K	649.81	Joback Method
cpg	378.69	J/mol×K	677.36	Joback Method
dvisc	0.0261311	Pa×s	270.66	Joback Method
dvisc	0.0063628	Pa×s	310.89	Joback Method
dvisc	0.0021415	Pa×s	351.12	Joback Method
dvisc	0.0009017	Pa×s	391.35	Joback Method
dvisc	0.0004461	Pa×s	431.59	Joback Method
dvisc	0.0002488	Pa×s	471.82	Joback Method
dvisc	0.0001521	Pa×s	512.05	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23144527&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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