2-Propanol, 1-chloro-3-(1-naphthalenyloxy)-

Other names: 1-Chloro-3-(1-naphthoxy)-2-propanol
1(Naphth-1-yloxy)-3-chlor-propan-2-ol
1-(Naphth-1-yloxy)-3-chloro-propan-2-ol
1-Chloro-3-(1-naphthyloxy)-2-propanol
2-Propanol, 1-chloro-3-(1-naphthyloxy)-
1-chloro-3-(1-naphthyloxy)propan-2-ol
Inchi: InChI=1S/C13H13ClO2/c14-8-11(15)9-16-13-7-3-5-10-4-1-2-6-12(10)13/h1-7,11,15H,8-9
InchiKey: ZVVJOJMCXYDDEW-UHFFFAOYSA-N
Formula: C13H13ClO2
SMILES: OC(CCl)COc1cccc2ccccc12
Mol. weight [g/mol]: 236.69
CAS: 20133-93-1

Physical Properties

Property code	Value	Unit	Source
gf	11.82	kJ/mol	Joback Method
hf	-200.99	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.818		Crippen Method
mcvol	174.790	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	699.07	K	Joback Method
tc	913.27	K	Joback Method
tf	405.88	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.20	J/mol×K	699.07	Joback Method
cpg	497.40	J/mol×K	877.57	Joback Method
cpg	488.55	J/mol×K	841.87	Joback Method

cpg	479.05	J/mol×K	806.17	Joback Method
cpg	468.86	J/mol×K	770.47	Joback Method
cpg	457.93	J/mol×K	734.77	Joback Method
cpg	505.68	J/mol×K	913.27	Joback Method
dvisc	0.0000611	Pa×s	699.07	Joback Method
dvisc	0.0000868	Pa×s	650.21	Joback Method
dvisc	0.0001306	Pa×s	601.34	Joback Method
dvisc	0.0002112	Pa×s	552.48	Joback Method
dvisc	0.0003751	Pa×s	503.61	Joback Method
dvisc	0.0007537	Pa×s	454.75	Joback Method
dvisc	0.0017913	Pa×s	405.88	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20133931&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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