1-Naphthalenol, 2,4-dichloro-

Other names: 1-Naphthol, 2,4-dichloro-
2,4-Dichloro-«alpha»-naphthol
2,4-Dichloro-1-naphthol
2,4-Dichloronaphthol
Inchi: InChI=1S/C10H6Cl2O/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5,13H
InchiKey: HVLJEMXDXOTWLV-UHFFFAOYSA-N
Formula: C10H6Cl2O
SMILES: Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]: 213.06
CAS: 2050-76-2

Physical Properties

Property code	Value	Unit	Source
gf	54.64	kJ/mol	Joback Method
hf	-53.86	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.852		Crippen Method
mcvol	138.890	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
rinpol	1648.00		NIST Webbook
tb	639.30	K	Joback Method
tc	898.93	K	Joback Method
tf	458.18	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.92	J/mol×K	639.30	Joback Method
cpg	336.03	J/mol×K	855.66	Joback Method
cpg	329.13	J/mol×K	812.38	Joback Method
cpg	321.92	J/mol×K	769.11	Joback Method

cpg	314.25	J/mol×K	725.84	Joback Method
cpg	305.97	J/mol×K	682.57	Joback Method
cpg	342.78	J/mol×K	898.93	Joback Method
dvisc	0.0000511	Pa×s	639.30	Joback Method
dvisc	0.0000683	Pa×s	609.11	Joback Method
dvisc	0.0000941	Pa×s	578.93	Joback Method
dvisc	0.0001343	Pa×s	548.74	Joback Method
dvisc	0.0001997	Pa×s	518.55	Joback Method
dvisc	0.0003120	Pa×s	488.37	Joback Method
dvisc	0.0005168	Pa×s	458.18	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=C2050762&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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