1-Naphthoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C14H11ClO2/c15-9-4-10-17-14(16)13-8-3-6-11-5-1-2-7-12(11)13/h1-9H,10H2/
InchiKey: OAUXYJNCYQYCJW-RUDMXATFSA-N
Formula: C14H11ClO2
SMILES: O=C(OCC=CCl)c1cccc2ccccc12
Mol. weight [g/mol]: 246.69

Physical Properties

Property code	Value	Unit	Source
gf	110.80	kJ/mol	Joback Method
hf	-59.48	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.749		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1999.00		NIST Webbook
tb	688.24	K	Joback Method
tc	926.66	K	Joback Method
tf	416.18	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.22	J/mol×K	688.24	Joback Method
cpg	448.98	J/mol×K	727.98	Joback Method
cpg	460.76	J/mol×K	767.71	Joback Method
cpg	471.65	J/mol×K	807.45	Joback Method
cpg	481.72	J/mol×K	847.18	Joback Method
cpg	491.06	J/mol×K	886.92	Joback Method
cpg	499.77	J/mol×K	926.66	Joback Method
dvisc	0.0012189	Pa×s	416.18	Joback Method
dvisc	0.0007915	Pa×s	461.52	Joback Method

dvisc	0.0005552	Pa×s	506.87	Joback Method
dvisc	0.0004128	Pa×s	552.21	Joback Method
dvisc	0.0003211	Pa×s	597.55	Joback Method
dvisc	0.0002587	Pa×s	642.90	Joback Method
dvisc	0.0002145	Pa×s	688.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308828&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