Propanamide, N-(1-naphthyl)-2-chloro-

Inchi: InChI=1S/C13H12ClNO/c1-9(14)13(16)15-12-8-4-6-10-5-2-3-7-11(10)12/h2-9H,1H3,(H,1
InchiKey: HZEXEFBFZFWVOD-UHFFFAOYSA-N
Formula: C13H12ClNO
SMILES: CC(Cl)C(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]: 233.69

Physical Properties

Property code	Value	Unit	Source
gf	214.11	kJ/mol	Joback Method
hf	24.35	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	66.29	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.406		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	688.51	K	Joback Method
tc	928.04	K	Joback Method
tf	425.42	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.02	J/mol×K	688.51	Joback Method
cpg	446.98	J/mol×K	728.43	Joback Method
cpg	458.91	J/mol×K	768.35	Joback Method
cpg	469.90	J/mol×K	808.28	Joback Method
cpg	480.04	J/mol×K	848.20	Joback Method
cpg	489.41	J/mol×K	888.12	Joback Method
cpg	498.11	J/mol×K	928.04	Joback Method

Sources

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=U307491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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