Propanamide, N-(1-naphthyl)-3-chloro-

Inchi: InChI=1S/C13H12ClNO/c14-9-8-13(16)15-12-7-3-5-10-4-1-2-6-11(10)12/h1-7H,8-9H2,(H
InchiKey: ISEAPHXDUWABSS-UHFFFAOYSA-N
Formula: C13H12ClNO
SMILES: O=C(CCCl)Nc1cccc2ccccc12
Mol. weight [g/mol]: 233.69

Physical Properties

Property code	Value	Unit	Source
gf	216.55	kJ/mol	Joback Method
hf	29.63	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.407		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	688.95	K	Joback Method
tc	923.73	K	Joback Method
tf	440.42	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.45	J/mol×K	688.95	Joback Method
cpg	446.13	J/mol×K	728.08	Joback Method
cpg	457.84	J/mol×K	767.21	Joback Method
cpg	468.64	J/mol×K	806.34	Joback Method
cpg	478.64	J/mol×K	845.47	Joback Method
cpg	487.91	J/mol×K	884.60	Joback Method
cpg	496.54	J/mol×K	923.73	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=U307232&Units=SI

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