Pentanamide, N-(1-naphthyl)-5-chloro-

Inchi: InChI=1S/C15H16ClNO/c16-11-4-3-10-15(18)17-14-9-5-7-12-6-1-2-8-13(12)14/h1-2,5-9H
InchiKey: ICQIPXNEVQEEDC-UHFFFAOYSA-N
Formula: C15H16ClNO
SMILES: O=C(CCCCCl)Nc1cccc2ccccc12
Mol. weight [g/mol]: 261.75

Physical Properties

Property code	Value	Unit	Source
gf	233.39	kJ/mol	Joback Method
hf	-11.65	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	71.13	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.187		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	2391.00		NIST Webbook
tb	734.71	K	Joback Method
tc	960.97	K	Joback Method
tf	462.96	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.67	J/mol×K	734.71	Joback Method
cpg	550.32	J/mol×K	772.42	Joback Method
cpg	563.00	J/mol×K	810.13	Joback Method
cpg	574.79	J/mol×K	847.84	Joback Method
cpg	585.77	J/mol×K	885.55	Joback Method
cpg	596.03	J/mol×K	923.26	Joback Method
cpg	605.65	J/mol×K	960.97	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=U307365&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