Benzamide, N-(1-naphthyl)-4-chloro-

Inchi: InChI=1S/C17H12ClNO/c18-14-10-8-13(9-11-14)17(20)19-16-7-3-5-12-4-1-2-6-15(12)16
InchiKey: IQWRPJFSMOZFIL-UHFFFAOYSA-N
Formula: C17H12ClNO
SMILES: O=C(Nc1cccc2ccccc12)c1ccc(Cl)cc1
Mol. weight [g/mol]: 281.74

Physical Properties

Property code	Value	Unit	Source
gf	353.01	kJ/mol	Joback Method
hf	172.13	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	78.52	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.745		Crippen Method
mcvol	207.200	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		NIST Webbook
tb	812.13	K	Joback Method
tc	1071.62	K	Joback Method
tf	524.44	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.08	J/mol×K	812.13	Joback Method
cpg	561.65	J/mol×K	855.38	Joback Method
cpg	573.14	J/mol×K	898.63	Joback Method
cpg	583.69	J/mol×K	941.87	Joback Method
cpg	593.45	J/mol×K	985.12	Joback Method
cpg	602.53	J/mol×K	1028.37	Joback Method
cpg	611.10	J/mol×K	1071.62	Joback Method

Sources

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=U307402&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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