

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

Inchi: InChI=1S/C18H15NO2/c1-21-15-11-9-14(10-12-15)18(20)19-17-8-4-6-13-5-2-3-7-16(13)
InchiKey: OHTOZIGJSMXGDB-UHFFFAOYSA-N
Formula: C18H15NO2
SMILES: COc1ccc(C(=O)Nc2cccc3ccccc23)cc1
Mol. weight [g/mol]: 277.32

Physical Properties

Property code	Value	Unit	Source
gf	268.36	kJ/mol	Joback Method
hf	35.01	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	78.77	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.101		Crippen Method
mcvol	214.920	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	820.00	K	Joback Method
tc	1068.62	K	Joback Method
tf	528.02	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.83	J/mol×K	820.00	Joback Method
cpg	620.53	J/mol×K	861.44	Joback Method
cpg	633.08	J/mol×K	902.87	Joback Method
cpg	644.55	J/mol×K	944.31	Joback Method
cpg	655.05	J/mol×K	985.75	Joback Method
cpg	664.69	J/mol×K	1027.18	Joback Method
cpg	673.55	J/mol×K	1068.62	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=U307502&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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