

Benzamide, n-methyl-n-phenyl-

Other names:	Benzanilide, N-methyl- N-Methyl-N-benzoylaniline N-Methylbenzoylaniline N-Methyl-N-phenylbenzamide N-Phenyl-N-methylbenzamide N-methylbenzanilide
Inchi:	InChI=1S/C14H13NO/c1-15(13-10-6-3-7-11-13)14(16)12-8-4-2-5-9-12/h2-11H,1H3
InchiKey:	LCOPCEDFGGUYRD-UHFFFAOYSA-N
Formula:	C14H13NO
SMILES:	CN(C(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	211.26

Physical Properties

Property code	Value	Unit	Source
af	0.5518		Cheméo Relay (1.0)
gf	273.68	kJ/mol	Joback Method
hf	37.26	kJ/mol	Cheméo Relay (1.0)
hfus	24.72	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-3.15		Cheméo Relay (1.0)
logp	2.963		Crippen Method
mcvol	172.150	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1771.97		NIST Webbook
rinpol	1814.08		NIST Webbook
rinpol	1819.97		NIST Webbook
rinpol	1771.97		NIST Webbook
tb	605.92	K	Cheméo Relay (1.0)
tc	878.14	K	Cheméo Relay (1.0)
tf	334.73	K	Cheméo Relay (1.0)
vc	0.636	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.11	J/mol×K	639.39	Joback Method
cpg	444.23	J/mol×K	679.80	Joback Method
cpg	459.00	J/mol×K	720.21	Joback Method
cpg	472.50	J/mol×K	760.62	Joback Method
cpg	484.83	J/mol×K	801.03	Joback Method
cpg	496.08	J/mol×K	841.44	Joback Method
cpg	506.35	J/mol×K	881.85	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1934925&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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