

Benzamide, N-(3-nitrophenyl)-3-methoxy-

Inchi:	InChI=1S/C14H12N2O4/c1-20-13-7-2-4-10(8-13)14(17)15-11-5-3-6-12(9-11)16(18)19/h2
InchiKey:	ZPXMTBWLEIEEBP-UHFFFAOYSA-N
Formula:	C14H12N2O4
SMILES:	<chem>COc1cccc(C(=O)Nc2cccc([N+](=O)[O-])c2)c1</chem>
Mol. weight [g/mol]:	272.26

Physical Properties

Property code	Value	Unit	Source
gf	163.58	kJ/mol	Joback Method
hf	-84.26	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	84.82	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.856		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	861.34	K	Joback Method
tc	1119.41	K	Joback Method
tf	593.85	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.65	J/molxK	861.34	Joback Method
cpg	568.74	J/molxK	904.35	Joback Method
cpg	578.61	J/molxK	947.36	Joback Method
cpg	587.31	J/molxK	990.38	Joback Method
cpg	594.92	J/molxK	1033.39	Joback Method
cpg	601.48	J/molxK	1076.40	Joback Method
cpg	607.06	J/molxK	1119.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U306973&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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