Benzamide, N-(4-methoxyphenyl)-4-nitro-

Inchi: InChI=1S/C14H12N2O4/c1-20-13-8-4-11(5-9-13)15-14(17)10-2-6-12(7-3-10)16(18)19/h2
InchiKey: NARGSXJDVYTGBN-UHFFFAOYSA-N
Formula: C14H12N2O4
SMILES: COc1ccc(NC(=O)c2ccc([N+](=O)[O-])cc2)cc1
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/mol×K	861.34	Joback Method
cpg	568.74	J/mol×K	904.35	Joback Method
cpg	578.61	J/mol×K	947.36	Joback Method
cpg	587.31	J/mol×K	990.38	Joback Method
cpg	594.92	J/mol×K	1033.39	Joback Method
cpg	601.48	J/mol×K	1076.40	Joback Method
cpg	607.06	J/mol×K	1119.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307353&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume