Benzamide, N-(3-methylphenyl)-4-nitro-

Inchi: InChI=1S/C14H12N2O3/c1-10-3-2-4-12(9-10)15-14(17)11-5-7-13(8-6-11)16(18)19/h2-9H
InchiKey: OJZGTNXZLKZWDC-UHFFFAOYSA-N
Formula: C14H12N2O3
SMILES: Cc1cccc(NC(=O)c2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]: 256.26

Physical Properties

Property code	Value	Unit	Source
gf	268.58	kJ/mol	Joback Method
hf	47.96	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.156		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	838.92	K	Joback Method
tc	1101.14	K	Joback Method
tf	571.62	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.12	J/mol×K	838.92	Joback Method
cpg	544.78	J/mol×K	882.62	Joback Method
cpg	555.28	J/mol×K	926.33	Joback Method
cpg	564.72	J/mol×K	970.03	Joback Method
cpg	573.17	J/mol×K	1013.74	Joback Method
cpg	580.72	J/mol×K	1057.44	Joback Method
cpg	587.48	J/mol×K	1101.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307351&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
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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