Benzamide, N-(2-iodo-4-methylphenyl)-4-nitro-

Inchi: InChI=1S/C14H11IN2O3/c1-9-2-7-13(12(15)8-9)16-14(18)10-3-5-11(6-4-10)17(19)20/h2-
InchiKey: UZIOLBOQDAUFBI-UHFFFAOYSA-N
Formula: C14H11IN2O3
SMILES: Cc1ccc(NC(=O)c2ccc([N+](=O)[O-])cc2)c(I)c1
Mol. weight [g/mol]: 382.15

Physical Properties

Property code	Value	Unit	Source
gf	317.07	kJ/mol	Joback Method
hf	113.36	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	92.44	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	3.760		Crippen Method
mcvol	215.390	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	2955.00		NIST Webbook
tb	937.04	K	Joback Method
tc	1220.51	K	Joback Method
tf	642.20	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.20	J/mol×K	937.04	Joback Method
cpg	573.78	J/mol×K	984.29	Joback Method
cpg	582.37	J/mol×K	1031.53	Joback Method
cpg	590.11	J/mol×K	1078.78	Joback Method
cpg	597.11	J/mol×K	1126.02	Joback Method
cpg	603.50	J/mol×K	1173.27	Joback Method
cpg	609.40	J/mol×K	1220.51	Joback Method

Sources

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=U307355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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