Acetamide, N-(3-nitrophenyl)-2-phenyl-

Inchi: InChI=1S/C14H12N2O3/c17-14(9-11-5-2-1-3-6-11)15-12-7-4-8-13(10-12)16(18)19/h1-8,1
InchiKey: NMZIQRANVSSSFS-UHFFFAOYSA-N
Formula: C14H12N2O3
SMILES: O=C(Cc1ccccc1)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 256.26

Physical Properties

Property code	Value	Unit	Source
gf	278.21	kJ/mol	Joback Method
hf	59.43	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	81.74	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.776		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	833.94	K	Joback Method
tc	1095.49	K	Joback Method
tf	559.10	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.84	J/mol×K	833.94	Joback Method
cpg	546.58	J/mol×K	877.53	Joback Method
cpg	557.16	J/mol×K	921.12	Joback Method
cpg	566.67	J/mol×K	964.71	Joback Method
cpg	575.21	J/mol×K	1008.30	Joback Method
cpg	582.88	J/mol×K	1051.89	Joback Method
cpg	589.79	J/mol×K	1095.49	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=U307147&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