Propanamide, N-(3-nitrophenyl)-3-phenyl-

Inchi: InChI=1S/C15H14N2O3/c18-15(10-9-12-5-2-1-3-6-12)16-13-7-4-8-14(11-13)17(19)20/h1
InchiKey: SRFQIDSDNDEYGS-UHFFFAOYSA-N
Formula: C15H14N2O3
SMILES: O=C(CCc1ccccc1)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
gf	286.63	kJ/mol	Joback Method
hf	38.79	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.166		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	2560.00		NIST Webbook
tb	856.82	K	Joback Method
tc	1113.04	K	Joback Method
tf	570.37	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.19	J/mol×K	856.82	Joback Method
cpg	601.25	J/mol×K	899.52	Joback Method
cpg	612.15	J/mol×K	942.23	Joback Method
cpg	622.00	J/mol×K	984.93	Joback Method
cpg	630.89	J/mol×K	1027.63	Joback Method
cpg	638.93	J/mol×K	1070.33	Joback Method
cpg	646.22	J/mol×K	1113.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308120&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