N-(4-Nitrophenyl)-N'-phenyl-urea

Other names: Urea, N-(4-nitrophenyl)-N'-phenyl-
Inchi: InChI=1S/C13H11N3O3/c17-13(14-10-4-2-1-3-5-10)15-11-6-8-12(9-7-11)16(18)19/h1-9H
InchiKey: QHHPMKKJBURYIQ-UHFFFAOYSA-N
Formula: C13H11N3O3
SMILES: O=C(Nc1ccccc1)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 257.24
CAS: 1932-32-7

Physical Properties

Property code	Value	Unit	Source
gf	359.18	kJ/mol	Joback Method
hf	133.54	kJ/mol	Joback Method
hfus	40.28	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.239		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	861.23	K	Joback Method
tc	1124.12	K	Joback Method
tf	600.49	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.25	J/mol×K	861.23	Joback Method
cpg	539.79	J/mol×K	905.05	Joback Method
cpg	549.21	J/mol×K	948.86	Joback Method
cpg	557.63	J/mol×K	992.68	Joback Method
cpg	565.15	J/mol×K	1036.49	Joback Method
cpg	571.86	J/mol×K	1080.31	Joback Method
cpg	577.86	J/mol×K	1124.12	Joback Method

Sources

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=C1932327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/70-040-9/N-4-Nitrophenyl-N-phenyl-urea.pdf
Generated by Cheméo on 2024-10-12 07:18:47.576442141 +0000 UTC m=+3298390.213411391.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.