Octanamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C14H20N2O3/c1-2-3-4-5-6-10-14(17)15-12-8-7-9-13(11-12)16(18)19/h7-9,11H
InchiKey: VADNAHSWKRFMHD-UHFFFAOYSA-N
Formula: C14H20N2O3
SMILES: CCCCCCCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	165.80	kJ/mol	Joback Method
hf	-177.10	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.894		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	807.26	K	Joback Method
tc	1030.28	K	Joback Method
tf	532.68	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.56	J/mol×K	807.26	Joback Method
cpg	645.22	J/mol×K	844.43	Joback Method
cpg	657.88	J/mol×K	881.60	Joback Method
cpg	669.59	J/mol×K	918.77	Joback Method
cpg	680.42	J/mol×K	955.94	Joback Method
cpg	690.41	J/mol×K	993.11	Joback Method
cpg	699.62	J/mol×K	1030.28	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=U306929&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume