Hexanamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C12H16N2O3/c1-2-3-4-8-12(15)13-10-6-5-7-11(9-10)14(16)17/h5-7,9H,2-4,8H
InchiKey: MPVGXCSUZCMVCI-UHFFFAOYSA-N
Formula: C12H16N2O3
SMILES: CCCCCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	148.96	kJ/mol	Joback Method
hf	-135.82	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.114		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	761.50	K	Joback Method
tc	991.13	K	Joback Method
tf	510.14	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.01	J/mol×K	761.50	Joback Method
cpg	535.96	J/mol×K	799.77	Joback Method
cpg	547.94	J/mol×K	838.04	Joback Method
cpg	558.99	J/mol×K	876.31	Joback Method
cpg	569.16	J/mol×K	914.58	Joback Method
cpg	578.52	J/mol×K	952.85	Joback Method
cpg	587.11	J/mol×K	991.13	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=U307292&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