Cyclohexanecarboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C13H16N2O3/c16-13(10-5-2-1-3-6-10)14-11-7-4-8-12(9-11)15(17)18/h4,7-10H
InchiKey: NXZZAYCXUXBWPA-UHFFFAOYSA-N
Formula: C13H16N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C1CCCCC1
Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
gf	181.83	kJ/mol	Joback Method
hf	-102.14	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.114		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	803.93	K	Joback Method
tc	1064.17	K	Joback Method
tf	528.79	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.97	J/mol×K	803.93	Joback Method
cpg	583.98	J/mol×K	847.30	Joback Method
cpg	597.52	J/mol×K	890.68	Joback Method
cpg	609.66	J/mol×K	934.05	Joback Method
cpg	620.50	J/mol×K	977.42	Joback Method
cpg	630.13	J/mol×K	1020.80	Joback Method
cpg	638.62	J/mol×K	1064.17	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=U306951&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