Cyclobutanecarboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C11H12N2O3/c14-11(8-3-1-4-8)12-9-5-2-6-10(7-9)13(15)16/h2,5-8H,1,3-4H2,(
InchiKey: YGYICSAGQSYTID-UHFFFAOYSA-N
Formula: C11H12N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C1CCC1
Mol. weight [g/mol]: 220.22

Physical Properties

Property code	Value	Unit	Source
gf	189.19	kJ/mol	Joback Method
hf	-48.54	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.333		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	2139.00		NIST Webbook
tb	749.63	K	Joback Method
tc	1006.02	K	Joback Method
tf	513.29	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.15	J/mol×K	749.63	Joback Method
cpg	469.39	J/mol×K	792.36	Joback Method
cpg	481.46	J/mol×K	835.09	Joback Method
cpg	492.46	J/mol×K	877.83	Joback Method
cpg	502.50	J/mol×K	920.56	Joback Method
cpg	511.67	J/mol×K	963.29	Joback Method
cpg	520.06	J/mol×K	1006.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307052&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