Cyclopentanecarboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C12H14N2O3/c15-12(9-4-1-2-5-9)13-10-6-3-7-11(8-10)14(16)17/h3,6-9H,1-2,4
InchiKey: YOMYHKWKZLGNIO-UHFFFAOYSA-N
Formula: C12H14N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C1CCCC1
Mol. weight [g/mol]: 234.25

Physical Properties

Property code	Value	Unit	Source
gf	185.51	kJ/mol	Joback Method
hf	-75.34	kJ/mol	Joback Method
hfus	32.48	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.723		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	776.78	K	Joback Method
tc	1035.16	K	Joback Method
tf	521.04	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.74	J/mol×K	776.78	Joback Method
cpg	525.97	J/mol×K	819.84	Joback Method
cpg	538.88	J/mol×K	862.91	Joback Method
cpg	550.57	J/mol×K	905.97	Joback Method
cpg	561.12	J/mol×K	949.03	Joback Method
cpg	570.65	J/mol×K	992.10	Joback Method
cpg	579.23	J/mol×K	1035.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307030&Units=SI

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