Cyclobutanecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H11NO4/c13-11(8-2-1-3-8)16-10-6-4-9(5-7-10)12(14)15/h4-8H,1-3H2
InchiKey: ATLCVECBGGXGAJ-UHFFFAOYSA-N
Formula: C11H11NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C1CCC1
Mol. weight [g/mol]: 221.21

Physical Properties

Property code	Value	Unit	Source
gf	-5.20	kJ/mol	Joback Method
hf	-234.23	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.300		Crippen Method
mcvol	156.090	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	721.88	K	Joback Method
tc	977.92	K	Joback Method
tf	482.86	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.57	J/mol×K	721.88	Joback Method
cpg	445.15	J/mol×K	764.55	Joback Method
cpg	457.55	J/mol×K	807.23	Joback Method
cpg	468.82	J/mol×K	849.90	Joback Method
cpg	479.03	J/mol×K	892.57	Joback Method
cpg	488.26	J/mol×K	935.24	Joback Method
cpg	496.57	J/mol×K	977.92	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=U307442&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