Cyclopropanecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C10H9NO4/c12-10(7-1-2-7)15-9-5-3-8(4-6-9)11(13)14/h3-7H,1-2H2

InchiKey: KYHAMGAANHSNPQ-UHFFFAOYSA-N

Formula: C10H9NO4

SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C1CC1

Mol. weight [g/mol]: 207.18

Physical Properties

Property code	Value	Unit	Source
gf	-1.52	kJ/mol	Joback Method
hf	-207.43	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.910		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1695.00		NIST Webbook
tb	694.73	K	Joback Method
tc	948.47	K	Joback Method
tf	475.11	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.87	J/mol×K	694.73	Joback Method
cpg	391.17	J/mol×K	737.02	Joback Method
cpg	402.43	J/mol×K	779.31	Joback Method
cpg	412.71	J/mol×K	821.60	Joback Method
cpg	422.11	J/mol×K	863.89	Joback Method
cpg	430.69	J/mol×K	906.18	Joback Method
cpg	438.52	J/mol×K	948.47	Joback Method

Sources

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=U307527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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