Cyclopropanecarboxylic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C11H9NO2/c12-7-8-1-5-10(6-2-8)14-11(13)9-3-4-9/h1-2,5-6,9H,3-4H2
InchiKey: GDMSAIHUURVTDC-UHFFFAOYSA-N
Formula: C11H9NO2
SMILES: N#Cc1ccc(OC(=O)C2CC2)cc1
Mol. weight [g/mol]: 187.19

Physical Properties

Property code	Value	Unit	Source
gf	104.53	kJ/mol	Joback Method
hf	-52.43	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	62.56	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.874		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	667.85	K	Joback Method
tc	907.57	K	Joback Method
tf	407.76	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.92	J/mol×K	667.85	Joback Method
cpg	366.67	J/mol×K	707.80	Joback Method
cpg	377.52	J/mol×K	747.76	Joback Method
cpg	387.54	J/mol×K	787.71	Joback Method
cpg	396.77	J/mol×K	827.66	Joback Method
cpg	405.27	J/mol×K	867.62	Joback Method
cpg	413.11	J/mol×K	907.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307525&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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