4-cyanobenzoic acid, cyclobutyl ester

Inchi: InChI=1S/C12H11NO2/c13-8-9-4-6-10(7-5-9)12(14)15-11-2-1-3-11/h4-7,11H,1-3H2
InchiKey: ZEYMYKZTNSCNKB-UHFFFAOYSA-N
Formula: C12H11NO2
SMILES: N#Cc1ccc(C(=O)OC2CCC2)cc1
Mol. weight [g/mol]: 201.23

Physical Properties

Property code	Value	Unit	Source
hf	-169.24	kJ/mol	Cheméo Relay (1.0)
hfus	20.82	kJ/mol	Joback Method
ie	9.85	eV	Cheméo Relay (1.0)
logp	2.268		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
rinpol	1692.60		NIST Webbook
rinpol	1692.60		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.42	J/mol×K	695.00	Joback Method
cpg	419.54	J/mol×K	735.39	Joback Method
cpg	431.63	J/mol×K	775.78	Joback Method
cpg	442.75	J/mol×K	816.17	Joback Method
cpg	452.93	J/mol×K	856.56	Joback Method
cpg	462.24	J/mol×K	896.95	Joback Method
cpg	470.72	J/mol×K	937.34	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292447&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices