4-cyanobenzoic acid, 2-adamantyl ester

Inchi: InChI=1S/C18H19NO2/c19-10-11-1-3-14(4-2-11)18(20)21-17-15-6-12-5-13(8-15)9-16(17
InchiKey: QDBHVGKGAUDWQE-UHFFFAOYSA-N
Formula: C18H19NO2
SMILES: N#Cc1ccc(C(=O)OC2C3CC4CC(C3)CC2C4)cc1
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
hfus	34.77	kJ/mol	Joback Method
ie	9.48	eV	Cheméo Relay (1.0)
logp	3.540		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
rinpol	2339.50		NIST Webbook
rinpol	2339.50		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.82	J/mol×K	836.42	Joback Method
cpg	721.31	J/mol×K	877.01	Joback Method
cpg	736.63	J/mol×K	917.60	Joback Method
cpg	750.92	J/mol×K	958.19	Joback Method
cpg	764.32	J/mol×K	998.78	Joback Method
cpg	776.97	J/mol×K	1039.37	Joback Method
cpg	789.00	J/mol×K	1079.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292449&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):	

Legend

cpg:	Ideal gas heat capacity
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