4-cyanobenzoic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C19H21NO2/c20-11-13-1-3-17(4-2-13)18(21)22-12-19-8-14-5-15(9-19)7-16(6-
InchiKey: YCAOTPGYMYJDPX-UHFFFAOYSA-N
Formula: C19H21NO2
SMILES: N#Cc1ccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 295.38

Physical Properties

Property code	Value	Unit	Source
hfus	29.99	kJ/mol	Joback Method
ie	9.45	eV	Cheméo Relay (1.0)
logp	3.931		Crippen Method
mcvol	231.050	ml/mol	McGowan Method
rinpol	2412.20		NIST Webbook
rinpol	2412.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.11	J/mol×K	864.21	Joback Method
cpg	773.88	J/mol×K	905.31	Joback Method
cpg	792.49	J/mol×K	946.41	Joback Method
cpg	811.21	J/mol×K	987.51	Joback Method
cpg	830.34	J/mol×K	1028.61	Joback Method
cpg	850.16	J/mol×K	1069.71	Joback Method
cpg	870.95	J/mol×K	1110.81	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=U292450&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
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