4-Cyanobenzoic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C20H23NO2/c21-13-14-1-3-18(4-2-14)19(22)23-6-5-20-10-15-7-16(11-20)9-17

InchiKey: AZWYYPCUJHQVSQ-UHFFFAOYSA-N

Formula: C20H23NO2

SMILES: N#Cc1ccc(C(=O)OCCC23CC4CC(CC(C4)C2)C3)cc1

Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
gf	276.51	kJ/mol	Joback Method
hf	-103.85	kJ/mol	Joback Method
hfus	32.58	kJ/mol	Joback Method
hvap	81.14	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.322		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	2509.00		NIST Webbook
rinpol	2509.00		NIST Webbook
tb	887.09	K	Joback Method
tc	1129.93	K	Joback Method
tf	561.21	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.46	J/mol×K	887.09	Joback Method
cpg	833.86	J/mol×K	927.56	Joback Method
cpg	853.18	J/mol×K	968.04	Joback Method
cpg	872.69	J/mol×K	1008.51	Joback Method
cpg	892.68	J/mol×K	1048.98	Joback Method
cpg	913.41	J/mol×K	1089.45	Joback Method
cpg	935.17	J/mol×K	1129.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292451&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