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
gf	257.45	kJ/mol	Joback Method
hf	-98.15	kJ/mol	Joback Method
hfus	34.77	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.540		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2339.50		NIST Webbook
rinpol	2339.50		NIST Webbook
tb	836.42	K	Joback Method
tc	1079.96	K	Joback Method
tf	510.53	K	Joback Method
vc	0.847	m3/kmol	Joback Method

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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