1-Adamantanecarboxylic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C18H19NO2/c19-11-12-1-3-16(4-2-12)21-17(20)18-8-13-5-14(9-18)7-15(6-13)
InchiKey: XCBOWRSWXPITOO-UHFFFAOYSA-N
Formula: C18H19NO2
SMILES: N#Cc1ccc(OC(=O)C23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
gf	259.67	kJ/mol	Joback Method
hf	-62.57	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	76.69	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.680		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
tb	841.33	K	Joback Method
tc	1092.36	K	Joback Method
tf	538.67	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.88	J/mol×K	841.33	Joback Method
cpg	715.05	J/mol×K	883.17	Joback Method
cpg	732.96	J/mol×K	925.01	Joback Method
cpg	750.92	J/mol×K	966.85	Joback Method
cpg	769.22	J/mol×K	1008.68	Joback Method
cpg	788.15	J/mol×K	1050.52	Joback Method
cpg	808.01	J/mol×K	1092.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307663&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

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