1-Adamantanecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C17H19NO4/c19-16(22-15-3-1-14(2-4-15)18(20)21)17-8-11-5-12(9-17)7-13(6-
InchiKey: UMKLOSVMOXTTNX-UHFFFAOYSA-N
Formula: C17H19NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 301.34

Physical Properties

Property code	Value	Unit	Source
gf	153.62	kJ/mol	Joback Method
hf	-217.57	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.717		Crippen Method
mcvol	218.910	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	868.21	K	Joback Method
tc	1131.05	K	Joback Method
tf	606.02	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.22	J/mol×K	868.21	Joback Method
cpg	745.27	J/mol×K	912.02	Joback Method
cpg	764.21	J/mol×K	955.82	Joback Method
cpg	783.38	J/mol×K	999.63	Joback Method
cpg	803.12	J/mol×K	1043.44	Joback Method
cpg	823.79	J/mol×K	1087.25	Joback Method
cpg	845.73	J/mol×K	1131.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307665&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