1-Adamantanecarboxylic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C18H22O3/c1-20-15-2-4-16(5-3-15)21-17(19)18-9-12-6-13(10-18)8-14(7-12)11

InchiKey: IISGTOWMMIBYLB-UHFFFAOYSA-N

Formula: C18H22O3

SMILES: COc1ccc(OC(=O)C23CC4CC(CC(C4)C2)C3)cc1

Mol. weight [g/mol]: 286.37

Physical Properties

Property code	Value	Unit	Source
gf	21.49	kJ/mol	Joback Method
hf	-359.67	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.817		Crippen Method
mcvol	221.450	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2314.00		NIST Webbook
tb	761.67	K	Joback Method
tc	999.87	K	Joback Method
tf	495.91	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.55	J/mol×K	761.67	Joback Method
cpg	715.56	J/mol×K	801.37	Joback Method
cpg	734.70	J/mol×K	841.07	Joback Method
cpg	753.22	J/mol×K	880.77	Joback Method
cpg	771.34	J/mol×K	920.47	Joback Method
cpg	789.30	J/mol×K	960.17	Joback Method
cpg	807.34	J/mol×K	999.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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