1-Adamantylmethyl 4-methoxyphenyl ketone

Inchi: InChI=1S/C19H24O2/c1-21-17-4-2-16(3-5-17)18(20)12-19-9-13-6-14(10-19)8-15(7-13)11
InchiKey: STPKFTIYXWZWGS-CSVIQDERSA-N
Formula: C19H24O2
SMILES: COc1ccc(C(=O)CC23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	134.91	kJ/mol	Joback Method
hf	-248.09	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.484		Crippen Method
mcvol	229.670	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	762.13	K	Joback Method
tc	999.19	K	Joback Method
tf	484.95	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.41	J/mol×K	762.13	Joback Method
cpg	744.17	J/mol×K	801.64	Joback Method
cpg	764.07	J/mol×K	841.15	Joback Method
cpg	783.36	J/mol×K	880.66	Joback Method
cpg	802.29	J/mol×K	920.17	Joback Method
cpg	821.11	J/mol×K	959.68	Joback Method
cpg	840.10	J/mol×K	999.19	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=R555690&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