1-Adamantyl phenyl ketone

Inchi: InChI=1S/C17H20O/c18-16(15-4-2-1-3-5-15)17-9-12-6-13(10-17)8-14(7-12)11-17/h1-5,1
InchiKey: IYXCOHWIYKULSE-ZZNDEYBLSA-N
Formula: C17H20O
SMILES: O=C(c1ccccc1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
gf	232.70	kJ/mol	Joback Method
hf	-63.12	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	60.91	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.086		Crippen Method
mcvol	195.620	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	688.97	K	Joback Method
tc	939.12	K	Joback Method
tf	427.66	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.86	J/mol×K	688.97	Joback Method
cpg	603.75	J/mol×K	730.66	Joback Method
cpg	623.35	J/mol×K	772.35	Joback Method
cpg	641.99	J/mol×K	814.05	Joback Method
cpg	659.98	J/mol×K	855.74	Joback Method
cpg	677.66	J/mol×K	897.43	Joback Method
cpg	695.35	J/mol×K	939.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R555729&Units=SI

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