propyl-(1-adamantyl) ketone

Other names: n-Propyladamantyl ketone
Inchi: InChI=1S/C14H22O/c1-2-3-13(15)14-7-10-4-11(8-14)6-12(5-10)9-14/h10-12H,2-9H2,1H3
InchiKey: VOYMPFHXYJTPFH-XHMIPKSJSA-N
Formula: C14H22O
SMILES: CCCC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	95.03	kJ/mol	Joback Method
hf	-237.73	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.572		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1641.00		NIST Webbook
ripol	2085.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2085.00		NIST Webbook
tb	593.65	K	Joback Method
tc	811.38	K	Joback Method
tf	367.43	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.50	J/mol×K	593.65	Joback Method

cpg	519.09	J/mol×K	629.94	Joback Method
cpg	538.32	J/mol×K	666.23	Joback Method
cpg	556.38	J/mol×K	702.51	Joback Method
cpg	573.48	J/mol×K	738.80	Joback Method
cpg	589.79	J/mol×K	775.09	Joback Method
cpg	605.53	J/mol×K	811.38	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=R189169&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume