ethyl-(1-adamantyl) ketone

Inchi: InChI=1S/C13H20O/c1-2-12(14)13-6-9-3-10(7-13)5-11(4-9)8-13/h9-11H,2-8H2,1H3
InchiKey: CUQIZWVVFUGCDM-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CCC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	86.61	kJ/mol	Joback Method
hf	-217.09	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.73	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.182		Crippen Method
mcvol	163.020	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1547.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2022.00		NIST Webbook
tb	570.77	K	Joback Method
tc	792.44	K	Joback Method
tf	356.16	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.92	J/mol×K	570.77	Joback Method
cpg	467.25	J/mol×K	607.71	Joback Method

cpg	486.13	J/mol×K	644.66	Joback Method
cpg	503.77	J/mol×K	681.60	Joback Method
cpg	520.37	J/mol×K	718.55	Joback Method
cpg	536.12	J/mol×K	755.49	Joback Method
cpg	551.24	J/mol×K	792.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304853&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

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