methyl-(2-adamantyl) ketone

Inchi: InChI=1S/C12H18O/c1-7(13)12-10-3-8-2-9(5-10)6-11(12)4-8/h8-12H,2-6H2,1H3
InchiKey: SAQHGEILSGZDQP-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(=O)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	75.97	kJ/mol	Joback Method
hf	-232.03	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.648		Crippen Method
mcvol	148.930	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1474.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1458.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1987.00		NIST Webbook
ripol	1939.00		NIST Webbook
tb	542.98	K	Joback Method
tc	759.64	K	Joback Method
tf	316.75	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.20	J/mol×K	542.98	Joback Method
cpg	418.85	J/mol×K	579.09	Joback Method

cpg	438.11	J/mol×K	615.20	Joback Method
cpg	456.08	J/mol×K	651.31	Joback Method
cpg	472.84	J/mol×K	687.42	Joback Method
cpg	488.50	J/mol×K	723.53	Joback Method
cpg	503.14	J/mol×K	759.64	Joback Method
dvisc	0.0018845	Pa×s	316.75	Joback Method
dvisc	0.0019772	Pa×s	354.45	Joback Method
dvisc	0.0020554	Pa×s	392.16	Joback Method
dvisc	0.0021222	Pa×s	429.87	Joback Method
dvisc	0.0021799	Pa×s	467.57	Joback Method
dvisc	0.0022302	Pa×s	505.28	Joback Method
dvisc	0.0022745	Pa×s	542.98	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=R304868&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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