Ethanone, 1-cyclododecyl-

Other names:	Ketone, cyclododecyl methyl
	1-Cyclododecylethanone
	Acetylcyclododecane
	1-Cyclododecylethan-1-one
	Cyclododecyl methyl ketone
Inchi:	InChI=1S/C14H26O/c1-13(15)14-11-9-7-5-3-2-4-6-8-10-12-14/h14H,2-12H2,1H3
InchiKey:	FTPUBZGARRXJIM-UHFFFAOYSA-N
Formula:	C14H26O
SMILES:	CC(=O)C1CCCCCCCCCCC1
Mol. weight [g/mol]:	210.36
CAS:	28925-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-110.07	kJ/mol	Joback Method
hf	-427.51	kJ/mol	Joback Method
hfus	12.85	kJ/mol	Joback Method
hvap	54.97	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.496		Crippen Method
mcvol	198.830	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1683.30		NIST Webbook
rinpol	1645.60		NIST Webbook
ripol	2067.30		NIST Webbook
ripol	2134.90		NIST Webbook
tb	618.76	K	Joback Method
tc	857.22	K	Joback Method
tf	283.73	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	543.80	J/mol×K	618.76	Joback Method
cpg	659.96	J/mol×K	817.48	Joback Method
cpg	640.35	J/mol×K	777.74	Joback Method
cpg	618.92	J/mol×K	737.99	Joback Method
cpg	595.68	J/mol×K	698.25	Joback Method
cpg	570.63	J/mol×K	658.50	Joback Method
cpg	677.73	J/mol×K	857.22	Joback Method
dvisc	0.0000391	Pa×s	618.76	Joback Method
dvisc	0.0000662	Pa×s	562.92	Joback Method
dvisc	0.0001256	Pa×s	507.08	Joback Method
dvisc	0.0002797	Pa×s	451.25	Joback Method
dvisc	0.0007805	Pa×s	395.41	Joback Method
dvisc	0.0030527	Pa×s	339.57	Joback Method
dvisc	0.0204220	Pa×s	283.73	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28925000&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
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