

Cyclohexanone, 2-ethyl-

Other names:	2-Ethylcyclohexanone
Inchi:	InChI=1S/C8H14O/c1-2-7-5-3-4-6-8(7)9/h7H,2-6H2,1H3
InchiKey:	WKYYYUWKFPFVEY-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CCC1CCCCC1=O
Mol. weight [g/mol]:	126.20
CAS:	4423-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-81.66	kJ/mol	Joback Method
hf	-291.83	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	38.08	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	469.81	K	Joback Method
tc	690.17	K	Joback Method
tf	255.52	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.75	J/mol×K	469.81	Joback Method
cpg	263.69	J/mol×K	506.54	Joback Method
cpg	279.88	J/mol×K	543.26	Joback Method
cpg	295.31	J/mol×K	579.99	Joback Method
cpg	309.98	J/mol×K	616.71	Joback Method

cpg	323.89	J/mol×K	653.44	Joback Method
cpg	337.02	J/mol×K	690.17	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=C4423943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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

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