

Cyclopentanone, 2-ethyl-

Other names:	2-Ethylcyclopentanone 2-ethylcyclopentan-1-one
Inchi:	InChI=1S/C7H12O/c1-2-6-4-3-5-7(6)8/h6H,2-5H2,1H3
InchiKey:	PPTKUTYPOKHBTL-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CCC1CCCC1=O
Mol. weight [g/mol]:	112.17
CAS:	4971-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-77.98	kJ/mol	Joback Method
hf	-265.03	kJ/mol	Joback Method
hfus	7.33	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
ripol	1314.00		NIST Webbook
tb	442.66	K	Joback Method
tc	657.51	K	Joback Method
tf	247.77	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.10	J/mol×K	442.66	Joback Method
cpg	219.78	J/mol×K	478.47	Joback Method
cpg	233.83	J/mol×K	514.28	Joback Method
cpg	247.27	J/mol×K	550.08	Joback Method
cpg	260.08	J/mol×K	585.89	Joback Method
cpg	272.27	J/mol×K	621.70	Joback Method

Sources

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=C4971180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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