

2-Ethoxy-2-cyclohexen-1-one

Other names:	2-Ethoxy-2-cyclohexenone 2-Cyclohexen-1-one, 2-ethoxy- 2-ethoxycyclohex-2-en-1-one
Inchi:	InChI=1S/C8H12O2/c1-2-10-8-6-4-3-5-7(8)9/h6H,2-5H2,1H3
InchiKey:	PJLUWPNLDKJSCF-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CCOC1=CCCCC1=O
Mol. weight [g/mol]:	140.18
CAS:	29941-82-0

Physical Properties

Property code	Value	Unit	Source
gf	-158.62	kJ/mol	Joback Method
hf	-357.40	kJ/mol	Joback Method
hfus	8.77	kJ/mol	Joback Method
hvap	41.75	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	501.04	K	Joback Method
tc	722.96	K	Joback Method
tf	295.27	K	Joback Method
vc	0.428	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.61	J/mol×K	501.04	Joback Method
cpg	269.18	J/mol×K	538.03	Joback Method
cpg	283.15	J/mol×K	575.01	Joback Method
cpg	296.49	J/mol×K	612.00	Joback Method
cpg	309.19	J/mol×K	648.98	Joback Method
cpg	321.22	J/mol×K	685.97	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=C29941820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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