2-ethyltetrahydro-3-furanone

Inchi: InChI=1S/C6H10O2/c1-2-6-5(7)3-4-8-6/h6H,2-4H2,1H3
InchiKey: MMVNDIYODKMKAF-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CCC1OCCC1=O
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
gf	-172.52	kJ/mol	Joback Method
hf	-376.39	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.754		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
ripol	1328.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1328.00		NIST Webbook
tb	446.73	K	Joback Method
tc	663.70	K	Joback Method
tf	263.07	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.05	J/mol×K	446.73	Joback Method
cpg	206.06	J/mol×K	482.89	Joback Method
cpg	218.55	J/mol×K	519.05	Joback Method
cpg	230.49	J/mol×K	555.22	Joback Method
cpg	241.89	J/mol×K	591.38	Joback Method
cpg	252.73	J/mol×K	627.54	Joback Method

cpg	263.02	J/mol×K	663.70	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=R491546&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
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