

2-Oxopropyl

Other names:	CH2COCH3
Inchi:	InChI=1S/C3H5O/c1-3(2)/h1H2,2H3
InchiKey:	HNUKTDKISXPDPA-UHFFFAOYSA-N
Formula:	C3H5O
SMILES:	[CH2]C(C)=O
Mol. weight [g/mol]:	57.07
CAS:	3122-07-4

Physical Properties

Property code	Value	Unit	Source
affp	820.00	kJ/mol	NIST Webbook
basg	787.50	kJ/mol	NIST Webbook
gf	-102.16	kJ/mol	Joback Method
hf	-162.02	kJ/mol	Joback Method
hfus	6.81	kJ/mol	Joback Method
hvap	28.87	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	0.409		Crippen Method
mcvol	52.550	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
tb	321.21	K	Joback Method
tc	496.10	K	Joback Method
tf	189.87	K	Joback Method
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.27	J/mol×K	321.21	Joback Method
cpg	79.67	J/mol×K	350.36	Joback Method
cpg	84.75	J/mol×K	379.51	Joback Method
cpg	89.50	J/mol×K	408.65	Joback Method
cpg	93.96	J/mol×K	437.80	Joback Method
cpg	98.13	J/mol×K	466.95	Joback Method

cpg	102.05	J/mol×K	496.10	Joback Method
dvisc	0.0006124	Pa×s	189.87	Joback Method
dvisc	0.0004966	Pa×s	211.76	Joback Method
dvisc	0.0004188	Pa×s	233.65	Joback Method
dvisc	0.0003637	Pa×s	255.54	Joback Method
dvisc	0.0003229	Pa×s	277.43	Joback Method
dvisc	0.0002918	Pa×s	299.32	Joback Method
dvisc	0.0002673	Pa×s	321.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3122074&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

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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