Propanedial

Inchi: InChI=1S/C3H4O2/c4-2-1-3-5/h2-3H,1H2
InchiKey: WSMYVTOQOOLQHP-UHFFFAOYSA-N
Formula: C3H4O2
SMILES: O=CCC=O
Mol. weight [g/mol]: 72.06
CAS: 542-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-224.66	kJ/mol	Joback Method
hf	-276.41	kJ/mol	Joback Method
hfus	8.10	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	0.36		Crippen Method
logp	-0.226		Crippen Method
mcvol	56.270	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	365.36	K	Joback Method
tc	548.24	K	Joback Method
tf	207.57	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.09	J/mol×K	365.36	Joback Method
cpg	98.70	J/mol×K	395.84	Joback Method
cpg	103.12	J/mol×K	426.32	Joback Method
cpg	107.36	J/mol×K	456.80	Joback Method
cpg	111.41	J/mol×K	487.28	Joback Method
cpg	115.29	J/mol×K	517.76	Joback Method
cpg	118.99	J/mol×K	548.24	Joback Method
dvisc	0.0029178	Pa×s	207.57	Joback Method
dvisc	0.0017176	Pa×s	233.87	Joback Method

dvisc	0.0011254	Pa×s	260.17	Joback Method
dvisc	0.0007969	Pa×s	286.47	Joback Method
dvisc	0.0005980	Pa×s	312.76	Joback Method
dvisc	0.0004692	Pa×s	339.06	Joback Method
dvisc	0.0003812	Pa×s	365.36	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542789&Units=SI

Legend

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