

Propylene ozonide

Other names:	Decomposes at source temperatures above 80 C
Inchi:	InChI=1S/C3H6O3/c1-3-4-2-5-6-3/h3H,2H2,1H3
InchiKey:	IZHVFAKMAKGJLM-UHFFFAOYSA-N
Formula:	C3H6O3
SMILES:	CC1OCCO1
Mol. weight [g/mol]:	90.08
CAS:	38787-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-349.26	kJ/mol	Joback Method
hf	-475.57	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	33.93	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.268		Crippen Method
mccvol	59.880	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	355.68	K	Joback Method
tc	540.41	K	Joback Method
tf	213.93	K	Joback Method
vc	0.215	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.34	J/molxK	355.68	Joback Method
cpg	109.72	J/molxK	386.47	Joback Method
cpg	115.72	J/molxK	417.26	Joback Method
cpg	121.37	J/molxK	448.05	Joback Method
cpg	126.68	J/molxK	478.84	Joback Method
cpg	131.67	J/molxK	509.62	Joback Method
cpg	136.34	J/molxK	540.41	Joback Method
dvisc	0.0010667	Paxs	213.93	Joback Method

dvisc	0.0008532	Paxs	237.56	Joback Method
dvisc	0.0007106	Paxs	261.18	Joback Method
dvisc	0.0006101	Paxs	284.81	Joback Method
dvisc	0.0005362	Paxs	308.43	Joback Method
dvisc	0.0004799	Paxs	332.06	Joback Method
dvisc	0.0004360	Paxs	355.68	Joback Method
hvapt	36.90	kJ/mol	278.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C38787961&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
hvapt:	Enthalpy of vaporization at a given temperature
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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