

Propanoic acid, 2-methyl-, anhydride

Other names:	Isobutyric anhydride Isobutryic anhydride Isobutyric acid anhydride Isobutyryl anhydride 2-Methylpropanoic anhydride (iso-C3H7CO)2O 2-Methylpropanoic acid anhydride UN 2530 Propanoic acid, 2-methyl-, 1,1'-anhydride
Inchi:	InChI=1S/C8H14O3/c1-5(2)7(9)11-8(10)6(3)4/h5-6H,1-4H3
InchiKey:	LSACYLWPPQLVSM-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CC(C)C(=O)OC(=O)C(C)C
Mol. weight [g/mol]:	158.19
CAS:	97-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-351.24	kJ/mol	Joback Method
hf	-576.39	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.368		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	455.20	K	NIST Webbook
tc	704.36	K	Joback Method
tf	272.01	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	299.22	J/mol×K	511.72	Joback Method
cpg	311.43	J/mol×K	543.83	Joback Method
cpg	323.13	J/mol×K	575.93	Joback Method
cpg	334.31	J/mol×K	608.04	Joback Method
cpg	344.97	J/mol×K	640.15	Joback Method
cpg	355.12	J/mol×K	672.25	Joback Method
cpg	364.75	J/mol×K	704.36	Joback Method
dvisc	0.0051001	Pa×s	272.01	Joback Method
dvisc	0.0022334	Pa×s	311.96	Joback Method
dvisc	0.0011797	Pa×s	351.91	Joback Method
dvisc	0.0007098	Pa×s	391.87	Joback Method
dvisc	0.0004691	Pa×s	431.82	Joback Method
dvisc	0.0003326	Pa×s	471.77	Joback Method
dvisc	0.0002488	Pa×s	511.72	Joback Method

Sources

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=C97723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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