Isobutyric 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]:	158.20

Physical Properties

Property code	Value	Unit	Source
af	0.5293		Cheméo Relay (1.0)
hf	-713.36	kJ/mol	Cheméo Relay (1.0)
hfus	13.82	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
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	610.23	K	Cheméo Relay (1.0)
tf	247.15	K	Cheméo Relay (1.0)
vc	0.512	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97723&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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