2,2-Dimethylpropanoic anhydride

Other names:	Trimethylacetic anhydride
	Pivalic anhydride
	Pivalic anydride
	Propanoic acid, 2,2-dimethyl-, anhydride
Inchi:	InChI=1S/C10H18O3/c1-9(2,3)7(11)13-8(12)10(4,5)6/h1-6H3
InchiKey:	PGZVFRAEAAXREB-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CC(C)(C)C(=O)OC(=O)C(C)(C)C
Mol. weight [g/mol]:	186.25
CAS:	1538-75-6

Physical Properties

Property code	Value	Unit	Source
gf	-323.84	kJ/mol	Joback Method
hf	-624.61	kJ/mol	Joback Method
hfus	11.21	kJ/mol	Joback Method
hvap	51.16	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.148		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1053.00		NIST Webbook
tb	466.20	K	NIST Webbook
tc	754.25	K	Joback Method
tf	329.39	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.18	J/mol×K	653.08	Joback Method
cpg	474.13	J/mol×K	754.25	Joback Method
cpg	463.24	J/mol×K	720.53	Joback Method
cpg	451.60	J/mol×K	686.80	Joback Method

cpg	396.75	J/mol×K	551.90	Joback Method
cpg	411.79	J/mol×K	585.63	Joback Method
cpg	425.92	J/mol×K	619.35	Joback Method
dvisc	0.0002020	Pa×s	551.90	Joback Method
dvisc	0.0005912	Pa×s	440.64	Joback Method
dvisc	0.0003910	Pa×s	477.73	Joback Method
dvisc	0.0002744	Pa×s	514.82	Joback Method
dvisc	0.0035749	Pa×s	329.39	Joback Method
dvisc	0.0017380	Pa×s	366.47	Joback Method
dvisc	0.0009647	Pa×s	403.56	Joback Method
hvapt	40.30 ± 0.70	kJ/mol	434.00	NIST Webbook
hvapt	44.00 ± 0.40	kJ/mol	434.00	NIST Webbook
hvapt	47.40 ± 0.20	kJ/mol	434.00	NIST Webbook
hvapt	50.70 ± 0.20	kJ/mol	434.00	NIST Webbook

Sources

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=C1538756&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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