

2-Methylbutanoic anhydride

Other names:	Isovaleric anhydride iso-Pentanoic anhydride Butanoic acid, 3-methyl-, anhydride
Inchi:	InChI=1S/C10H18O3/c1-7(2)5-9(11)13-10(12)6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	FREZLSIGWNCSEQ-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CC(C)CC(=O)OC(=O)CC(C)C
Mol. weight [g/mol]:	186.25
CAS:	1468-39-9

Physical Properties

Property code	Value	Unit	Source
gf	-334.40	kJ/mol	Joback Method
hf	-617.67	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.148		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	557.48	K	Joback Method
tc	745.50	K	Joback Method
tf	294.55	K	Joback Method
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.89	J/mol×K	557.48	Joback Method
cpg	404.87	J/mol×K	588.82	Joback Method
cpg	418.24	J/mol×K	620.15	Joback Method
cpg	430.98	J/mol×K	651.49	Joback Method
cpg	443.11	J/mol×K	682.83	Joback Method
cpg	454.64	J/mol×K	714.16	Joback Method

cpg	465.56	J/mol×K	745.50	Joback Method
dvisc	0.0046668	Paxs	294.55	Joback Method
dvisc	0.0019868	Paxs	338.37	Joback Method
dvisc	0.0010288	Paxs	382.19	Joback Method
dvisc	0.0006100	Paxs	426.01	Joback Method
dvisc	0.0003987	Paxs	469.84	Joback Method
dvisc	0.0002802	Paxs	513.66	Joback Method
dvisc	0.0002082	Paxs	557.48	Joback Method

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=C1468399&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

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