

Isovaleric 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

Physical Properties

Property code	Value	Unit	Source
af	0.6129		Cheméo Relay (1.0)
hf	-768.52	kJ/mol	Cheméo Relay (1.0)
hfus	19.00	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-2.69		Cheméo Relay (1.0)
logp	2.148		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	436.51	K	Cheméo Relay (1.0)
tc	650.30	K	Cheméo Relay (1.0)
tf	230.36	K	Cheméo Relay (1.0)

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	Pa×s	294.55	Joback Method
dvisc	0.0019868	Pa×s	338.37	Joback Method
dvisc	0.0010288	Pa×s	382.19	Joback Method
dvisc	0.0006100	Pa×s	426.01	Joback Method
dvisc	0.0003987	Pa×s	469.84	Joback Method
dvisc	0.0002802	Pa×s	513.66	Joback Method
dvisc	0.0002082	Pa×s	557.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1468399&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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