ISOAMYL ACETOACETATE

Other names:	Butanoic acid, 3-oxo-, 3-methylbutyl ester
	Isoamyl acetoacetate
	3-Methylbutyl 3-oxobutanoate
	Isoamyl acetylacetate
	Isoamyl «beta»-ketobutyrate
	Isopentyl «beta»-ketobutyrate
	isopentyl acetoacetate
Inchi:	InChI=1S/C9H16O3/c1-7(2)4-5-12-9(11)6-8(3)10/h7H,4-6H2,1-3H3
InchiKey:	XHRGPLDMNNGHCX-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CC(=O)CC(=O)OCCC(C)C
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
hf	-669.23	kJ/mol	Cheméo Relay (1.0)
hfus	19.93	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Cheméo Relay (1.0)
ie	9.40	eV	Cheméo Relay (1.0)
log10ws	-1.55		Cheméo Relay (1.0)
logp	1.555		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
tb	491.00	K	NIST Webbook
tc	670.89	K	Cheméo Relay (1.0)
tf	233.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.82	J/mol×K	535.04	Joback Method
cpg	356.65	J/mol×K	566.12	Joback Method
cpg	368.94	J/mol×K	597.19	Joback Method
cpg	380.69	J/mol×K	628.27	Joback Method

cpg	391.90	J/mol×K	659.35	Joback Method
cpg	402.58	J/mol×K	690.42	Joback Method
cpg	412.73	J/mol×K	721.50	Joback Method
dvisc	0.0035617	Pa×s	298.28	Joback Method
dvisc	0.0017528	Pa×s	337.74	Joback Method
dvisc	0.0010005	Pa×s	377.20	Joback Method
dvisc	0.0006351	Pa×s	416.66	Joback Method
dvisc	0.0004361	Pa×s	456.12	Joback Method
dvisc	0.0003180	Pa×s	495.58	Joback Method
dvisc	0.0002429	Pa×s	535.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2308181&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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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