BUTANOIC ACID, 3-OXO-, 2-METHYLPROPYL ESTER

Other names: 2-Methyl-1-propyl acetoacetate
Acetoacetic acid, isobutyl ester
Isobutyl 3-ketobutanoate
Isobutyl 3-ketobutyrate
Isobutyl acetoacetate

Inchi: InChI=1S/C8H14O3/c1-6(2)5-11-8(10)4-7(3)9/h6H,4-5H2,1-3H3

InchiKey: ZYXNLVMBIHVDRH-UHFFFAOYSA-N

Formula: C8H14O3

SMILES: CC(=O)CC(=O)OCC(C)C

Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
af	0.5374		Cheméo Relay (1.0)
hf	-654.20	kJ/mol	Cheméo Relay (1.0)
hfus	17.34	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-1.04		Cheméo Relay (1.0)
logp	1.165		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	477.00	K	NIST Webbook
tc	651.64	K	Cheméo Relay (1.0)
tf	241.56	K	Cheméo Relay (1.0)
vc	0.488	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.94	J/mol×K	512.16	Joback Method
cpg	362.98	J/mol×K	700.78	Joback Method

cpg	353.52	J/mol×K	669.35	Joback Method
cpg	343.58	J/mol×K	637.91	Joback Method
cpg	333.16	J/mol×K	606.47	Joback Method
cpg	322.24	J/mol×K	575.03	Joback Method
cpg	310.84	J/mol×K	543.60	Joback Method
dvisc	0.0006771	Pa×s	399.58	Joback Method
dvisc	0.0002635	Pa×s	512.16	Joback Method
dvisc	0.0003434	Pa×s	474.63	Joback Method
dvisc	0.0004683	Pa×s	437.11	Joback Method
dvisc	0.0036492	Pa×s	287.01	Joback Method
dvisc	0.0010567	Pa×s	362.06	Joback Method
dvisc	0.0018279	Pa×s	324.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	2.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779751&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume