SEC-BUTYL ACETOACETATE

Other names: Acetoacetic acid, sec-butyl ester
sec-Butyl Acetoacetate
Inchi: InChI=1S/C8H14O3/c1-4-7(3)11-8(10)5-6(2)9/h7H,4-5H2,1-3H3
InchiKey: QSTNBMLCULGCQE-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCC(C)OC(=O)CC(C)=O
Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
hf	-670.30	kJ/mol	Cheméo Relay (1.0)
hfus	17.34	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Cheméo Relay (1.0)
ie	9.46	eV	Cheméo Relay (1.0)
logp	1.307		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
tb	467.00	K	NIST Webbook
tf	239.13	K	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	310.84	J/mol×K	543.60	Joback Method
cpg	322.24	J/mol×K	575.03	Joback Method
cpg	333.16	J/mol×K	606.47	Joback Method
cpg	343.58	J/mol×K	637.91	Joback Method
cpg	353.52	J/mol×K	669.35	Joback Method
cpg	362.98	J/mol×K	700.78	Joback Method
dvisc	0.0036492	Pa×s	287.01	Joback Method
dvisc	0.0018279	Pa×s	324.53	Joback Method
dvisc	0.0010567	Pa×s	362.06	Joback Method
dvisc	0.0006771	Pa×s	399.58	Joback Method
dvisc	0.0004683	Pa×s	437.11	Joback Method

dvisc	0.0003434	Pa×s	474.63	Joback Method
dvisc	0.0002635	Pa×s	512.16	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13562760&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

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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point