BUTANOIC ACID, 2,2-DIMETHYL-3-OXO-, ETHYL ESTER

Other names: ethyl 2,2-dimethylacetoacetate
ethyl 2,2-dimethyl-3-oxobutanoate
Inchi: InChI=1S/C8H14O3/c1-5-11-7(10)8(3,4)6(2)9/h5H2,1-4H3
InchiKey: NVAHZHOCRQCUBY-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCOC(=O)C(C)(C)C(C)=O
Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
af	0.4423		Cheméo Relay (1.0)
gf	-343.52	kJ/mol	Joback Method
hf	-650.92	kJ/mol	Cheméo Relay (1.0)
hfus	13.45	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-1.06		Cheméo Relay (1.0)
logp	1.165		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	452.37	K	Cheméo Relay (1.0)
tc	636.05	K	Cheméo Relay (1.0)
tf	267.71	K	Cheméo Relay (1.0)
vc	0.484	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.98	J/mol×K	509.37	Joback Method
cpg	314.46	J/mol×K	542.04	Joback Method
cpg	326.31	J/mol×K	574.70	Joback Method
cpg	337.53	J/mol×K	607.37	Joback Method
cpg	348.15	J/mol×K	640.04	Joback Method
cpg	358.18	J/mol×K	672.71	Joback Method

cpg	367.64	J/mol×K	705.37	Joback Method
dvisc	0.0033814	Pa×s	304.43	Joback Method
dvisc	0.0017905	Pa×s	338.59	Joback Method
dvisc	0.0010652	Pa×s	372.74	Joback Method
dvisc	0.0006915	Pa×s	406.90	Joback Method
dvisc	0.0004799	Pa×s	441.06	Joback Method
dvisc	0.0003511	Pa×s	475.21	Joback Method
dvisc	0.0002678	Pa×s	509.37	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C597046&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
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
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
vc: Critical Volume