Butanedioic acid, acetyl-, diethyl ester

Other names:	Diethyl acetylsuccinate
	Acetylsuccinic acid diethyl ester
	Diethyl acetosuccinate
	Diethyl 2-acetylsuccinate
	Ethyl acetylsuccinate
	Succinic acid, acetyl-, diethyl ester
Inchi:	InChI=1S/C10H16O5/c1-4-14-9(12)6-8(7(3)11)10(13)15-5-2/h8H,4-6H2,1-3H3
InchiKey:	DVSDDICSXBCMQJ-UHFFFAOYSA-N
Formula:	C10H16O5
SMILES:	CCOC(=O)CC(C(C)=O)C(=O)OCC
Mol. weight [g/mol]:	216.23
CAS:	1115-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-565.88	kJ/mol	Joback Method
hf	-857.19	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.708		Crippen Method
mcvol	168.210	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	528.20	K	NIST Webbook
tb	528.00 ± 1.00	K	NIST Webbook
tc	825.12	K	Joback Method
tf	381.71	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.27	J/mol×K	634.21	Joback Method
cpg	446.78	J/mol×K	666.03	Joback Method

cpg	458.67	J/mol×K	697.85	Joback Method
cpg	469.95	J/mol×K	729.67	Joback Method
cpg	480.59	J/mol×K	761.48	Joback Method
cpg	490.60	J/mol×K	793.30	Joback Method
cpg	499.97	J/mol×K	825.12	Joback Method
dvisc	0.0019096	Pa×s	381.71	Joback Method
dvisc	0.0010572	Pa×s	423.79	Joback Method
dvisc	0.0006513	Pa×s	465.88	Joback Method
dvisc	0.0004348	Pa×s	507.96	Joback Method
dvisc	0.0003088	Pa×s	550.04	Joback Method
dvisc	0.0002302	Pa×s	592.13	Joback Method
dvisc	0.0001784	Pa×s	634.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.70	K	6.70	NIST Webbook
tbrp	414.00 ± 1.00	K	2.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115306&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume