PENTANEDIOIC ACID, 2-ACETYL-, DIETHYL ESTER

Other names: Diethyl «alpha»-acetoglutarate
Diethyl «alpha»-acetylglutarate
Pentanedioic acid, 2-acetyl-, diethyl ester
2-Acetylglutaric acid, diethyl ester

Inchi: InChI=1S/C11H18O5/c1-4-15-10(13)7-6-9(8(3)12)11(14)16-5-2/h9H,4-7H2,1-3H3

InchiKey: NNOGMCQLKMLNPL-UHFFFAOYSA-N

Formula: C11H18O5

SMILES: CCOC(=O)CCC(C(C)=O)C(=O)OCC

Mol. weight [g/mol]: 230.26

Physical Properties

Property code	Value	Unit	Source
af	0.6580		Cheméo Relay (1.0)
gf	-557.46	kJ/mol	Joback Method
hf	-1020.67	kJ/mol	Cheméo Relay (1.0)
hfus	27.90	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-0.80		Cheméo Relay (1.0)
logp	1.098		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	544.50 ± 0.50	K	NIST Webbook
tc	719.56	K	Cheméo Relay (1.0)
tf	270.99	K	Cheméo Relay (1.0)
vc	0.664	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.73	J/mol×K	657.09	Joback Method
cpg	497.88	J/mol×K	688.60	Joback Method
cpg	510.36	J/mol×K	720.11	Joback Method
cpg	522.17	J/mol×K	751.62	Joback Method

cpg	533.31	J/mol×K	783.13	Joback Method
cpg	543.77	J/mol×K	814.64	Joback Method
cpg	553.55	J/mol×K	846.15	Joback Method
dvisc	0.0017853	Pa×s	392.98	Joback Method
dvisc	0.0009733	Pa×s	437.00	Joback Method
dvisc	0.0005929	Pa×s	481.02	Joback Method
dvisc	0.0003925	Pa×s	525.03	Joback Method
dvisc	0.0002770	Pa×s	569.05	Joback Method
dvisc	0.0002055	Pa×s	613.07	Joback Method
dvisc	0.0001586	Pa×s	657.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.20	K	1.50	NIST Webbook
tbrp	443.00 ± 1.00	K	2.90	NIST Webbook
tbrp	435.00	K	1.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501060&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):

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