ACETIC ACID, CYCLOHEXYLIDENE-, ETHYL ESTER

Other names: «delta»1,«alpha»-Cyclohexaneacetic acid, ethyl ester
Ethyl cyclohexylideneacetate
Ethoxycarbonylmethylenecyclohexane

Inchi: InChI=1S/C10H16O2/c1-2-12-10(11)8-9-6-4-3-5-7-9/h8H,2-7H2,1H3

InchiKey: MCWDXHYYYNGYGK-UHFFFAOYSA-N

Formula: C10H16O2

SMILES: CCOC(=O)C=C1CCCCC1

Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
af	0.4351		Cheméo Relay (1.0)
hf	-432.46	kJ/mol	Cheméo Relay (1.0)
hfus	15.53	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-2.98		Cheméo Relay (1.0)
logp	2.440		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	495.02	K	Cheméo Relay (1.0)
tc	696.28	K	Cheméo Relay (1.0)
tf	258.06	K	Cheméo Relay (1.0)
vc	0.505	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.78	J/mol×K	535.35	Joback Method
cpg	353.12	J/mol×K	570.74	Joback Method
cpg	368.57	J/mol×K	606.13	Joback Method
cpg	383.15	J/mol×K	641.52	Joback Method
cpg	396.90	J/mol×K	676.91	Joback Method
cpg	409.82	J/mol×K	712.30	Joback Method

cpg	421.95	J/mol×K	747.70	Joback Method
dvisc	0.0033197	Pa×s	296.60	Joback Method
dvisc	0.0015677	Pa×s	336.39	Joback Method
dvisc	0.0008677	Pa×s	376.18	Joback Method
dvisc	0.0005378	Pa×s	415.98	Joback Method
dvisc	0.0003623	Pa×s	455.77	Joback Method
dvisc	0.0002601	Pa×s	495.56	Joback Method
dvisc	0.0001962	Pa×s	535.35	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1552927&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
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

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