1,3-DIOXOLANE-2-ACETIC ACID, 2-METHYL-, ETHYL ESTER

Other names: 1,3-Dioxolane-2-acetic acid, 2-methyl-, ethyl ester
Ethyl acetoacetate ethylene ketal
Ethyl acetoacetate 3-ethylene acetal
Ethyl 2-methyl-1,3-dioxolane-2-acetate

Inchi: InChI=1S/C8H14O4/c1-3-10-7(9)6-8(2)11-4-5-12-8/h3-6H2,1-2H3

InchiKey: XWEOGMYZFCHQNT-UHFFFAOYSA-N

Formula: C8H14O4

SMILES: CCOC(=O)CC1(C)OCCO1

Mol. weight [g/mol]: 174.20

Physical Properties

Property code	Value	Unit	Source
af	0.4789		Cheméo Relay (1.0)
gf	-358.62	kJ/mol	Joback Method
hf	-790.72	kJ/mol	Cheméo Relay (1.0)
hfus	22.86	kJ/mol	Joback Method
hvap	60.75	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
log10ws	-0.66		Cheméo Relay (1.0)
logp	0.703		Crippen Method
mcvol	131.900	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1123.10		NIST Webbook
rinpol	1123.10		NIST Webbook
tb	461.29	K	Cheméo Relay (1.0)
tc	658.96	K	Cheméo Relay (1.0)
tf	235.46	K	Cheméo Relay (1.0)
vc	0.509	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.66	J/mol×K	528.15	Joback Method
cpg	337.53	J/mol×K	563.11	Joback Method

cpg	350.58	J/mol×K	598.07	Joback Method
cpg	362.89	J/mol×K	633.03	Joback Method
cpg	374.54	J/mol×K	667.98	Joback Method
cpg	385.62	J/mol×K	702.94	Joback Method
cpg	396.23	J/mol×K	737.90	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6413101&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.