Ethyl acetoacetate ethylene acetal

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]:	174.19
CAS:	6413-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-358.62	kJ/mol	Joback Method
hf	-641.53	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
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	528.15	K	Joback Method
tc	737.90	K	Joback Method
tf	340.02	K	Joback Method
vc	0.488	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6413101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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

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