

1,3-Dioxolane-2-propanoic acid, 2-methyl-, ethyl ester

Other names:	1,3-Dioxolane-2-propionic acid, 2-methyl-, ethyl ester 2-Propionic acid, 2-methyl-1,3-dioxolane-, ethyl ester ethyl 2-methyl-1,3-dioxolane-2-propionate
Inchi:	InChI=1S/C9H16O4/c1-3-11-8(10)4-5-9(2)12-6-7-13-9/h3-7H2,1-2H3
InchiKey:	PLUNGZQWVYCJBJ-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	CCOC(=O)CCC1(C)OCCO1
Mol. weight [g/mol]:	188.22
CAS:	941-43-5

Physical Properties

Property code	Value	Unit	Source
gf	-350.20	kJ/mol	Joback Method
hf	-662.17	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.093		Crippen Method
mcvol	145.990	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	551.03	K	Joback Method
tc	757.53	K	Joback Method
tf	351.29	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.75	J/molxK	551.03	Joback Method
cpg	384.41	J/molxK	585.45	Joback Method
cpg	398.24	J/molxK	619.86	Joback Method
cpg	411.33	J/molxK	654.28	Joback Method
cpg	423.77	J/molxK	688.70	Joback Method
cpg	435.63	J/molxK	723.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C941435&Units=SI

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
mccvol:	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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