Ethyl mesitylglyoxylate

Inchi:	InChI=1S/C13H16O3/c1-5-16-13(15)12(14)11-9(3)6-8(2)7-10(11)4/h6-7H,5H2,1-4H3
InchiKey:	XRSPPFOBPRPYLD-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	CCOC(=O)C(=O)c1c(C)cc(C)cc1C
Mol. weight [g/mol]:	220.26
CAS:	5524-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-220.74	kJ/mol	Joback Method
hf	-466.91	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.358		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	668.62	K	Joback Method
tc	881.13	K	Joback Method
tf	422.34	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.01	J/mol×K	668.62	Joback Method
cpg	521.36	J/mol×K	845.71	Joback Method
cpg	510.67	J/mol×K	810.29	Joback Method
cpg	499.20	J/mol×K	774.87	Joback Method
cpg	486.94	J/mol×K	739.46	Joback Method
cpg	473.87	J/mol×K	704.04	Joback Method
cpg	531.27	J/mol×K	881.13	Joback Method
dvisc	0.0001682	Pa×s	668.62	Joback Method
dvisc	0.0002052	Pa×s	627.57	Joback Method

dvisc	0.0002573	Pa×s	586.53	Joback Method
dvisc	0.0003337	Pa×s	545.48	Joback Method
dvisc	0.0004517	Pa×s	504.43	Joback Method
dvisc	0.0006450	Pa×s	463.39	Joback Method
dvisc	0.0009870	Pa×s	422.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5524572&Units=SI

Legend

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
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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