Diglycolic acid, ethyl 2-formylphenyl ester

Inchi: InChI=1S/C13H14O6/c1-2-18-12(15)8-17-9-13(16)19-11-6-4-3-5-10(11)7-14/h3-7H,2,8-9
InchiKey: GBOKTVHRCQQYET-UHFFFAOYSA-N
Formula: C13H14O6
SMILES: CCOC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 266.25

Physical Properties

Property code	Value	Unit	Source
gf	-511.00	kJ/mol	Joback Method
hf	-793.99	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	74.91	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.984		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	752.16	K	Joback Method
tc	961.58	K	Joback Method
tf	483.76	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.80	J/mol×K	752.16	Joback Method
cpg	578.39	J/mol×K	926.68	Joback Method
cpg	570.09	J/mol×K	891.78	Joback Method
cpg	560.88	J/mol×K	856.87	Joback Method
cpg	550.75	J/mol×K	821.97	Joback Method
cpg	539.72	J/mol×K	787.06	Joback Method
cpg	585.75	J/mol×K	961.58	Joback Method
dvisc	0.0001146	Pa×s	752.16	Joback Method

dvisc	0.0001422	Pa×s	707.43	Joback Method
dvisc	0.0001816	Pa×s	662.69	Joback Method
dvisc	0.0002404	Pa×s	617.96	Joback Method
dvisc	0.0003325	Pa×s	573.23	Joback Method
dvisc	0.0004859	Pa×s	528.49	Joback Method
dvisc	0.0007615	Pa×s	483.76	Joback Method

Sources

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=U382306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume