Diglycolic acid, di(2-formylphenyl) ester

Inchi: InChI=1S/C18H14O7/c19-9-13-5-1-3-7-15(13)24-17(21)11-23-12-18(22)25-16-8-4-2-6-14
InchiKey: QLKXZQWOINZWAT-UHFFFAOYSA-N
Formula: C18H14O7
SMILES: O=Cc1ccccc1OC(=O)COCC(=O)Oc1ccccc1C=O
Mol. weight [g/mol]: 342.30

Physical Properties

Property code	Value	Unit	Source
gf	-465.64	kJ/mol	Joback Method
hf	-757.71	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	95.70	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	1.839		Crippen Method
mcvol	240.850	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	3458.00		NIST Webbook
rinpol	3458.00		NIST Webbook
tb	946.88	K	Joback Method
tc	1179.94	K	Joback Method
tf	621.05	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.35	J/mol×K	946.88	Joback Method
cpg	717.07	J/mol×K	985.72	Joback Method
cpg	724.44	J/mol×K	1024.57	Joback Method
cpg	730.46	J/mol×K	1063.41	Joback Method
cpg	735.15	J/mol×K	1102.26	Joback Method
cpg	738.51	J/mol×K	1141.10	Joback Method
cpg	740.53	J/mol×K	1179.94	Joback Method
dvisc	0.0003929	Pa×s	621.05	Joback Method

dvisc	0.0002592	Pa×s	675.36	Joback Method
dvisc	0.0001819	Pa×s	729.66	Joback Method
dvisc	0.0001341	Pa×s	783.96	Joback Method
dvisc	0.0001028	Pa×s	838.27	Joback Method
dvisc	0.0000814	Pa×s	892.58	Joback Method
dvisc	0.0000662	Pa×s	946.88	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=U382314&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