Diglycolic acid, di(2-acetylphenyl) ester

Inchi: InChI=1S/C20H18O7/c1-13(21)15-7-3-5-9-17(15)26-19(23)11-25-12-20(24)27-18-10-6-4
InchiKey: VVMWPLAKJAFVAP-UHFFFAOYSA-N
Formula: C20H18O7
SMILES: CC(=O)c1ccccc1OC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 370.35

Physical Properties

Property code	Value	Unit	Source
gf	-507.60	kJ/mol	Joback Method
hf	-852.99	kJ/mol	Joback Method
hfus	44.82	kJ/mol	Joback Method
hvap	100.20	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	2.619		Crippen Method
mcvol	269.030	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	3205.00		NIST Webbook
rinpol	3205.00		NIST Webbook
tb	1003.06	K	Joback Method
tc	1240.69	K	Joback Method
tf	659.45	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.32	J/mol×K	1003.06	Joback Method
cpg	847.42	J/mol×K	1201.08	Joback Method
cpg	845.09	J/mol×K	1161.48	Joback Method
cpg	841.22	J/mol×K	1121.87	Joback Method
cpg	835.81	J/mol×K	1082.27	Joback Method
cpg	828.85	J/mol×K	1042.66	Joback Method
cpg	848.23	J/mol×K	1240.69	Joback Method
dvisc	0.0000390	Pa×s	1003.06	Joback Method

dvisc	0.0000482	Pa×s	945.79	Joback Method
dvisc	0.0000613	Pa×s	888.52	Joback Method
dvisc	0.0000804	Pa×s	831.25	Joback Method
dvisc	0.0001099	Pa×s	773.99	Joback Method
dvisc	0.0001579	Pa×s	716.72	Joback Method
dvisc	0.0002415	Pa×s	659.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382730&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
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