Diglycolic acid, di(2,5-dimethylphenyl) ester

Inchi: InChI=1S/C20H22O5/c1-13-5-7-15(3)17(9-13)24-19(21)11-23-12-20(22)25-18-10-14(2)6
InchiKey: ZPSTZMJWJCDNPU-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: Cc1ccc(C)c(OC(=O)COCC(=O)Oc2cc(C)ccc2C)c1
Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-269.02	kJ/mol	Joback Method
hf	-650.77	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.448		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	3179.00		NIST Webbook
rinpol	3179.00		NIST Webbook
tb	905.28	K	Joback Method
tc	1130.61	K	Joback Method
tf	584.63	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.07	J/mol×K	905.28	Joback Method
cpg	818.20	J/mol×K	942.83	Joback Method
cpg	829.91	J/mol×K	980.39	Joback Method
cpg	840.22	J/mol×K	1017.94	Joback Method
cpg	849.11	J/mol×K	1055.50	Joback Method
cpg	856.59	J/mol×K	1093.05	Joback Method
cpg	862.65	J/mol×K	1130.61	Joback Method
dvisc	0.0002603	Pa×s	584.63	Joback Method

dvisc	0.0001715	Pa×s	638.07	Joback Method
dvisc	0.0001205	Pa×s	691.51	Joback Method
dvisc	0.0000891	Pa×s	744.95	Joback Method
dvisc	0.0000685	Pa×s	798.40	Joback Method
dvisc	0.0000545	Pa×s	851.84	Joback Method
dvisc	0.0000445	Pa×s	905.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382715&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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