Diglycolic acid, di(phenethyl) ester

Inchi: InChI=1S/C20H22O5/c21-19(24-13-11-17-7-3-1-4-8-17)15-23-16-20(22)25-14-12-18-9-5
InchiKey: FWZJIESNNCLMAL-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: O=C(COCC(=O)OCCc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-230.50	kJ/mol	Joback Method
hf	-604.89	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.575		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	885.36	K	Joback Method
tc	1107.59	K	Joback Method
tf	534.55	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.91	J/mol×K	885.36	Joback Method
cpg	823.50	J/mol×K	922.40	Joback Method
cpg	835.74	J/mol×K	959.44	Joback Method
cpg	846.66	J/mol×K	996.48	Joback Method
cpg	856.29	J/mol×K	1033.51	Joback Method
cpg	864.66	J/mol×K	1070.55	Joback Method
cpg	871.79	J/mol×K	1107.59	Joback Method
dvisc	0.0004184	Pa×s	534.55	Joback Method

dvisc	0.0002354	Pa×s	593.02	Joback Method
dvisc	0.0001468	Pa×s	651.49	Joback Method
dvisc	0.0000990	Pa×s	709.96	Joback Method
dvisc	0.0000709	Pa×s	768.42	Joback Method
dvisc	0.0000532	Pa×s	826.89	Joback Method
dvisc	0.0000414	Pa×s	885.36	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=U382168&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