Diglycolic acid, octyl phenethyl ester

Inchi: InChI=1S/C20H30O5/c1-2-3-4-5-6-10-14-24-19(21)16-23-17-20(22)25-15-13-18-11-8-7-9
InchiKey: NVPMXCQYKLEGAZ-UHFFFAOYSA-N
Formula: C20H30O5
SMILES: CCCCCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-342.91	kJ/mol	Joback Method
hf	-841.42	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	83.11	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.693		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook
tb	858.68	K	Joback Method
tc	1059.32	K	Joback Method
tf	508.13	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.79	J/mol×K	858.68	Joback Method
cpg	923.53	J/mol×K	892.12	Joback Method
cpg	938.06	J/mol×K	925.56	Joback Method
cpg	951.40	J/mol×K	959.00	Joback Method
cpg	963.57	J/mol×K	992.44	Joback Method
cpg	974.58	J/mol×K	1025.88	Joback Method
cpg	984.46	J/mol×K	1059.32	Joback Method
dvisc	0.0004837	Pa×s	508.13	Joback Method

dvisc	0.0002586	Pa×s	566.55	Joback Method
dvisc	0.0001554	Pa×s	624.98	Joback Method
dvisc	0.0001019	Pa×s	683.40	Joback Method
dvisc	0.0000714	Pa×s	741.83	Joback Method
dvisc	0.0000527	Pa×s	800.25	Joback Method
dvisc	0.0000405	Pa×s	858.68	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=U382163&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