Diglycolic acid, heptyl phenethyl ester

Inchi: InChI=1S/C19H28O5/c1-2-3-4-5-9-13-23-18(20)15-22-16-19(21)24-14-12-17-10-7-6-8-11
InchiKey: IEJMSTJEWVWWNZ-UHFFFAOYSA-N
Formula: C19H28O5
SMILES: CCCCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-351.33	kJ/mol	Joback Method
hf	-820.78	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.302		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	3149.00		NIST Webbook
tb	835.80	K	Joback Method
tc	1035.35	K	Joback Method
tf	496.86	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.89	J/mol×K	835.80	Joback Method
cpg	915.23	J/mol×K	1002.09	Joback Method
cpg	904.21	J/mol×K	968.84	Joback Method
cpg	892.08	J/mol×K	935.58	Joback Method
cpg	878.82	J/mol×K	902.32	Joback Method
cpg	864.43	J/mol×K	869.06	Joback Method
cpg	925.15	J/mol×K	1035.35	Joback Method
dvisc	0.0000468	Pa×s	835.80	Joback Method
dvisc	0.0000607	Pa×s	779.31	Joback Method

dvisc	0.0000819	Pa×s	722.82	Joback Method
dvisc	0.0001163	Pa×s	666.33	Joback Method
dvisc	0.0001763	Pa×s	609.84	Joback Method
dvisc	0.0002909	Pa×s	553.35	Joback Method
dvisc	0.0005380	Pa×s	496.86	Joback Method

Sources

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=U382162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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