Diglycolic acid, 2,6-dimethoxyphenyl heptyl ester

Inchi: InChI=1S/C19H28O7/c1-4-5-6-7-8-12-25-17(20)13-24-14-18(21)26-19-15(22-2)10-9-11-1

InchiKey: OBXRDTPVPHLBDH-UHFFFAOYSA-N

Formula: C19H28O7

SMILES: CCCCCCCOC(=O)COCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 368.42

Physical Properties

Property code	Value	Unit	Source
gf	-580.59	kJ/mol	Joback Method
hf	-1108.16	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	87.03	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.139		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	3228.00		NIST Webbook
tb	890.60	K	Joback Method
tc	1095.42	K	Joback Method
tf	566.36	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.79	J/mol×K	890.60	Joback Method
cpg	919.03	J/mol×K	924.74	Joback Method
cpg	931.88	J/mol×K	958.87	Joback Method
cpg	943.32	J/mol×K	993.01	Joback Method
cpg	953.32	J/mol×K	1027.14	Joback Method
cpg	961.86	J/mol×K	1061.28	Joback Method
cpg	968.91	J/mol×K	1095.42	Joback Method
dvisc	0.0002015	Pa×s	566.36	Joback Method
dvisc	0.0001245	Pa×s	620.40	Joback Method

dvisc	0.0000830	Pa×s	674.44	Joback Method
dvisc	0.0000588	Pa×s	728.48	Joback Method
dvisc	0.0000437	Pa×s	782.52	Joback Method
dvisc	0.0000338	Pa×s	836.56	Joback Method
dvisc	0.0000269	Pa×s	890.60	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=U381909&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