Diglycolic acid, 2,6-dimethoxyphenyl hexyl ester

Inchi: InChI=1S/C18H26O7/c1-4-5-6-7-11-24-16(19)12-23-13-17(20)25-18-14(21-2)9-8-10-15(1

InchiKey: HFDRAMPSTHRARC-UHFFFAOYSA-N

Formula: C18H26O7

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

Mol. weight [g/mol]: 354.39

Physical Properties

Property code	Value	Unit	Source
gf	-589.01	kJ/mol	Joback Method
hf	-1087.52	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.749		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook
tb	867.72	K	Joback Method
tc	1070.81	K	Joback Method
tf	555.09	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.14	J/mol×K	867.72	Joback Method
cpg	903.55	J/mol×K	1036.96	Joback Method
cpg	894.77	J/mol×K	1003.11	Joback Method
cpg	884.62	J/mol×K	969.26	Joback Method
cpg	873.11	J/mol×K	935.42	Joback Method
cpg	860.28	J/mol×K	901.57	Joback Method
cpg	910.93	J/mol×K	1070.81	Joback Method
dvisc	0.0000311	Pa×s	867.72	Joback Method

dvisc	0.0000389	Pa×s	815.62	Joback Method
dvisc	0.0000501	Pa×s	763.51	Joback Method
dvisc	0.0000671	Pa×s	711.40	Joback Method
dvisc	0.0000940	Pa×s	659.30	Joback Method
dvisc	0.0001396	Pa×s	607.19	Joback Method
dvisc	0.0002234	Pa×s	555.09	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=U381908&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