Diglycolic acid, butyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C16H22O7/c1-4-5-9-22-14(17)10-21-11-15(18)23-16-12(19-2)7-6-8-13(16)20-3

InchiKey: DLUQDQUHLWYTPN-UHFFFAOYSA-N

Formula: C16H22O7

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

Mol. weight [g/mol]: 326.34

Physical Properties

Property code	Value	Unit	Source
gf	-605.85	kJ/mol	Joback Method
hf	-1046.24	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.969		Crippen Method
mcvol	245.030	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	821.96	K	Joback Method
tc	1023.82	K	Joback Method
tf	532.55	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.96	J/mol×K	821.96	Joback Method
cpg	744.77	J/mol×K	855.60	Joback Method
cpg	757.44	J/mol×K	889.25	Joback Method
cpg	768.94	J/mol×K	922.89	Joback Method
cpg	779.24	J/mol×K	956.53	Joback Method
cpg	788.31	J/mol×K	990.18	Joback Method
cpg	796.11	J/mol×K	1023.82	Joback Method
dvisc	0.0002711	Pa×s	532.55	Joback Method

dvisc	0.0001738	Pa×s	580.78	Joback Method
dvisc	0.0001193	Pa×s	629.02	Joback Method
dvisc	0.0000864	Pa×s	677.25	Joback Method
dvisc	0.0000653	Pa×s	725.49	Joback Method
dvisc	0.0000511	Pa×s	773.73	Joback Method
dvisc	0.0000412	Pa×s	821.96	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=U381905&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

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