Diglycolic acid, 2,6-dimethoxyphenyl isobutyl ester

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

InchiKey: QFOSOBYGBXTBHA-UHFFFAOYSA-N

Formula: C16H22O7

SMILES: COc1cccc(OC)c1OC(=O)COCC(=O)OCC(C)C

Mol. weight [g/mol]: 326.34

Physical Properties

Property code	Value	Unit	Source
gf	-608.29	kJ/mol	Joback Method
hf	-1051.52	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.825		Crippen Method
mcvol	245.030	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2801.00		NIST Webbook
rinpol	2801.00		NIST Webbook
tb	821.52	K	Joback Method
tc	1025.55	K	Joback Method
tf	517.55	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.51	J/mol×K	821.52	Joback Method
cpg	745.47	J/mol×K	855.52	Joback Method
cpg	758.24	J/mol×K	889.53	Joback Method
cpg	769.81	J/mol×K	923.53	Joback Method
cpg	780.14	J/mol×K	957.54	Joback Method
cpg	789.20	J/mol×K	991.54	Joback Method
cpg	796.96	J/mol×K	1025.55	Joback Method
dvisc	0.0002979	Pa×s	517.55	Joback Method

dvisc	0.0001811	Pa×s	568.21	Joback Method
dvisc	0.0001195	Pa×s	618.87	Joback Method
dvisc	0.0000839	Pa×s	669.53	Joback Method
dvisc	0.0000619	Pa×s	720.20	Joback Method
dvisc	0.0000476	Pa×s	770.86	Joback Method
dvisc	0.0000378	Pa×s	821.52	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=U381904&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

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