Diglycolic acid, butyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H24O6/c1-4-5-10-21-16(18)11-20-12-17(19)23-15-9-7-6-8-14(15)22-13(2)3

InchiKey: VLRXARNIVLBWIL-UHFFFAOYSA-N

Formula: C17H24O6

SMILES: CCCCOC(=O)COCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-485.24	kJ/mol	Joback Method
hf	-928.47	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	79.12	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.739		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2854.00		NIST Webbook
rinpol	2854.00		NIST Webbook
tb	817.00	K	Joback Method
tc	1019.65	K	Joback Method
tf	494.07	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.51	J/mol×K	817.00	Joback Method
cpg	823.53	J/mol×K	985.87	Joback Method
cpg	813.47	J/mol×K	952.10	Joback Method
cpg	802.23	J/mol×K	918.32	Joback Method
cpg	789.82	J/mol×K	884.55	Joback Method
cpg	776.24	J/mol×K	850.77	Joback Method
cpg	832.40	J/mol×K	1019.65	Joback Method
dvisc	0.0000432	Pa×s	817.00	Joback Method

dvisc	0.0000556	Pa×s	763.18	Joback Method
dvisc	0.0000742	Pa×s	709.36	Joback Method
dvisc	0.0001040	Pa×s	655.53	Joback Method
dvisc	0.0001547	Pa×s	601.71	Joback Method
dvisc	0.0002489	Pa×s	547.89	Joback Method
dvisc	0.0004441	Pa×s	494.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U381981&Units=SI

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