Diglycolic acid, di(4-methoxyphenyl) ester

Inchi: InChI=1S/C18H18O7/c1-21-13-3-7-15(8-4-13)24-17(19)11-23-12-18(20)25-16-9-5-14(22
InchiKey: FEXZECRQSUSOAE-UHFFFAOYSA-N
Formula: C18H18O7
SMILES: COc1ccc(OC(=O)COCC(=O)Oc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 346.33

Physical Properties

Property code	Value	Unit	Source
gf	-476.60	kJ/mol	Joback Method
hf	-850.99	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.231		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	3472.00		NIST Webbook
rinpol	3472.00		NIST Webbook
tb	894.40	K	Joback Method
tc	1119.50	K	Joback Method
tf	581.51	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.19	J/mol×K	894.40	Joback Method
cpg	757.93	J/mol×K	931.92	Joback Method
cpg	768.17	J/mol×K	969.43	Joback Method
cpg	776.87	J/mol×K	1006.95	Joback Method
cpg	783.99	J/mol×K	1044.46	Joback Method
cpg	789.53	J/mol×K	1081.98	Joback Method
cpg	793.44	J/mol×K	1119.50	Joback Method
dvisc	0.0002025	Pa×s	581.51	Joback Method

dvisc	0.0001311	Pa×s	633.66	Joback Method
dvisc	0.0000906	Pa×s	685.81	Joback Method
dvisc	0.0000660	Pa×s	737.95	Joback Method
dvisc	0.0000502	Pa×s	790.10	Joback Method
dvisc	0.0000394	Pa×s	842.25	Joback Method
dvisc	0.0000319	Pa×s	894.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381891&Units=SI
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

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