Diglycolic acid, 2-formylphenyl hexyl ester

Inchi: InChI=1S/C17H22O6/c1-2-3-4-7-10-22-16(19)12-21-13-17(20)23-15-9-6-5-8-14(15)11-18

InchiKey: QOWIVPJKPLMESD-UHFFFAOYSA-N

Formula: C17H22O6

SMILES: CCCCCCOC(=O)COCC(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-477.32	kJ/mol	Joback Method
hf	-876.55	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	83.82	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.545		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2967.00		NIST Webbook
rinpol	2967.00		NIST Webbook
tb	843.68	K	Joback Method
tc	1048.55	K	Joback Method
tf	528.84	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.82	J/mol×K	843.68	Joback Method
cpg	760.98	J/mol×K	877.82	Joback Method
cpg	773.05	J/mol×K	911.97	Joback Method
cpg	784.02	J/mol×K	946.11	Joback Method
cpg	793.91	J/mol×K	980.26	Joback Method
cpg	802.71	J/mol×K	1014.40	Joback Method
cpg	810.42	J/mol×K	1048.55	Joback Method
dvisc	0.0005393	Pa×s	528.84	Joback Method

dvisc	0.0003262	Pa×s	581.31	Joback Method
dvisc	0.0002145	Pa×s	633.79	Joback Method
dvisc	0.0001503	Pa×s	686.26	Joback Method
dvisc	0.0001109	Pa×s	738.73	Joback Method
dvisc	0.0000851	Pa×s	791.21	Joback Method
dvisc	0.0000675	Pa×s	843.68	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=U382312&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