Diglycolic acid, 2-formylphenyl isohexyl ester

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

InchiKey: OWUABLIVYLSIPM-UHFFFAOYSA-N

Formula: C17H22O6

SMILES: CC(C)CCCOC(=O)COCC(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-479.76	kJ/mol	Joback Method
hf	-881.83	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	83.43	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.401		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2917.00		NIST Webbook
rinpol	2917.00		NIST Webbook
tb	843.24	K	Joback Method
tc	1050.17	K	Joback Method
tf	513.84	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.37	J/mol×K	843.24	Joback Method
cpg	803.52	J/mol×K	1015.68	Joback Method
cpg	794.74	J/mol×K	981.20	Joback Method
cpg	784.83	J/mol×K	946.71	Joback Method
cpg	773.81	J/mol×K	912.22	Joback Method
cpg	761.65	J/mol×K	877.73	Joback Method
cpg	811.18	J/mol×K	1050.17	Joback Method
dvisc	0.0000619	Pa×s	843.24	Joback Method

dvisc	0.0000791	Pa×s	788.34	Joback Method
dvisc	0.0001051	Pa×s	733.44	Joback Method
dvisc	0.0001460	Pa×s	678.54	Joback Method
dvisc	0.0002150	Pa×s	623.64	Joback Method
dvisc	0.0003411	Pa×s	568.74	Joback Method
dvisc	0.0005973	Pa×s	513.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382311&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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