Diglycolic acid, isohexyl 2-isopropylphenyl ester

Inchi: InChI=1S/C19H28O5/c1-14(2)8-7-11-23-18(20)12-22-13-19(21)24-17-10-6-5-9-16(17)15

InchiKey: ATAVRMGZAICUFC-UHFFFAOYSA-N

Formula: C19H28O5

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

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-365.84	kJ/mol	Joback Method
hf	-842.81	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.711		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2774.00		NIST Webbook
rinpol	2774.00		NIST Webbook
tb	839.90	K	Joback Method
tc	1044.02	K	Joback Method
tf	479.38	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.22	J/mol×K	839.90	Joback Method
cpg	864.93	J/mol×K	873.92	Joback Method
cpg	879.43	J/mol×K	907.94	Joback Method
cpg	892.71	J/mol×K	941.96	Joback Method
cpg	904.79	J/mol×K	975.98	Joback Method
cpg	915.68	J/mol×K	1010.00	Joback Method
cpg	925.38	J/mol×K	1044.02	Joback Method
dvisc	0.0005924	Pa×s	479.38	Joback Method

dvisc	0.0002940	Pa×s	539.47	Joback Method
dvisc	0.0001679	Pa×s	599.55	Joback Method
dvisc	0.0001062	Pa×s	659.64	Joback Method
dvisc	0.0000725	Pa×s	719.73	Joback Method
dvisc	0.0000525	Pa×s	779.81	Joback Method
dvisc	0.0000398	Pa×s	839.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382290&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