Diglycolic acid, 2,5-dimethylphenyl pentyl ester

Inchi: InChI=1S/C17H24O5/c1-4-5-6-9-21-16(18)11-20-12-17(19)22-15-10-13(2)7-8-14(15)3/h7

InchiKey: XSJISICCBROPGT-UHFFFAOYSA-N

Formula: C17H24O5

SMILES: CCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-387.43	kJ/mol	Joback Method
hf	-802.44	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.959		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	800.00	K	Joback Method
tc	1001.07	K	Joback Method
tf	499.36	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.87	J/mol×K	800.00	Joback Method
cpg	746.79	J/mol×K	833.51	Joback Method
cpg	760.66	J/mol×K	867.02	Joback Method
cpg	773.48	J/mol×K	900.54	Joback Method
cpg	785.25	J/mol×K	934.05	Joback Method
cpg	795.95	J/mol×K	967.56	Joback Method
cpg	805.60	J/mol×K	1001.07	Joback Method
dvisc	0.0004802	Pa×s	499.36	Joback Method

dvisc	0.0002932	Pa×s	549.47	Joback Method
dvisc	0.0001945	Pa×s	599.57	Joback Method
dvisc	0.0001374	Pa×s	649.68	Joback Method
dvisc	0.0001020	Pa×s	699.79	Joback Method
dvisc	0.0000788	Pa×s	749.89	Joback Method
dvisc	0.0000629	Pa×s	800.00	Joback Method

Sources

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=U382706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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