Diglycolic acid, 2,5-dimethylphenyl octyl ester

Inchi: InChI=1S/C20H30O5/c1-4-5-6-7-8-9-12-24-19(21)14-23-15-20(22)25-18-13-16(2)10-11-1
InchiKey: NENONRKPRBQECF-UHFFFAOYSA-N
Formula: C20H30O5
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-362.17	kJ/mol	Joback Method
hf	-864.36	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.129		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	868.64	K	Joback Method
tc	1071.07	K	Joback Method
tf	533.17	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.40	J/mol×K	868.64	Joback Method
cpg	971.98	J/mol×K	1037.33	Joback Method
cpg	961.29	J/mol×K	1003.60	Joback Method
cpg	949.39	J/mol×K	969.86	Joback Method
cpg	936.28	J/mol×K	936.12	Joback Method
cpg	921.95	J/mol×K	902.38	Joback Method
cpg	981.47	J/mol×K	1071.07	Joback Method
dvisc	0.0000417	Pa×s	868.64	Joback Method

dvisc	0.0000528	Pa×s	812.73	Joback Method
dvisc	0.0000693	Pa×s	756.82	Joback Method
dvisc	0.0000949	Pa×s	700.90	Joback Method
dvisc	0.0001373	Pa×s	644.99	Joback Method
dvisc	0.0002129	Pa×s	589.08	Joback Method
dvisc	0.0003621	Pa×s	533.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382710&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