Diglycolic acid, decyl 2,5-dimethylphenyl ester

Inchi: InChI=1S/C22H34O5/c1-4-5-6-7-8-9-10-11-14-26-21(23)16-25-17-22(24)27-20-15-18(2)1
InchiKey: YBBXWOSIJWOQMD-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: CCCCCCCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-345.33	kJ/mol	Joback Method
hf	-905.64	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.909		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	3317.00		NIST Webbook
tb	914.40	K	Joback Method
tc	1121.51	K	Joback Method
tf	555.71	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.34	J/mol×K	914.40	Joback Method
cpg	1092.25	J/mol×K	1086.99	Joback Method
cpg	1081.77	J/mol×K	1052.47	Joback Method
cpg	1069.94	J/mol×K	1017.95	Joback Method
cpg	1056.77	J/mol×K	983.44	Joback Method
cpg	1042.24	J/mol×K	948.92	Joback Method
cpg	1101.41	J/mol×K	1121.51	Joback Method
dvisc	0.0000313	Pa×s	914.40	Joback Method
dvisc	0.0000399	Pa×s	854.62	Joback Method

dvisc	0.0000528	Pa×s	794.84	Joback Method
dvisc	0.0000730	Pa×s	735.05	Joback Method
dvisc	0.0001070	Pa×s	675.27	Joback Method
dvisc	0.0001688	Pa×s	615.49	Joback Method
dvisc	0.0002938	Pa×s	555.71	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=U382712&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