Diglycolic acid, heptyl 2-methylphenyl ester

Inchi: InChI=1S/C18H26O5/c1-3-4-5-6-9-12-22-17(19)13-21-14-18(20)23-16-11-8-7-10-15(16)2
InchiKey: RBJBOZOWIMATOB-UHFFFAOYSA-N
Formula: C18H26O5
SMILES: CCCCCCCOC(=O)COCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-369.38	kJ/mol	Joback Method
hf	-811.61	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	79.32	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.431		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	817.90	K	Joback Method
tc	1017.91	K	Joback Method
tf	498.11	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.00	J/mol×K	817.90	Joback Method
cpg	855.27	J/mol×K	984.57	Joback Method
cpg	844.40	J/mol×K	951.24	Joback Method
cpg	832.44	J/mol×K	917.90	Joback Method
cpg	819.39	J/mol×K	884.57	Joback Method
cpg	805.25	J/mol×K	851.23	Joback Method
cpg	865.06	J/mol×K	1017.91	Joback Method
dvisc	0.0000544	Pa×s	817.90	Joback Method

dvisc	0.0000694	Pa×s	764.60	Joback Method
dvisc	0.0000917	Pa×s	711.30	Joback Method
dvisc	0.0001268	Pa×s	658.00	Joback Method
dvisc	0.0001857	Pa×s	604.71	Joback Method
dvisc	0.0002926	Pa×s	551.41	Joback Method
dvisc	0.0005083	Pa×s	498.11	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=U382010&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