Diglycolic acid, butyl undecyl ester

Inchi: InChI=1S/C19H36O5/c1-3-5-7-8-9-10-11-12-13-15-24-19(21)17-22-16-18(20)23-14-6-4-2
InchiKey: KCEACNHSPGCWHW-UHFFFAOYSA-N
Formula: C19H36O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-463.74	kJ/mol	Joback Method
hf	-1057.31	kJ/mol	Joback Method
hfus	51.73	kJ/mol	Joback Method
hvap	78.61	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.420		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2905.00		NIST Webbook
rinpol	2905.00		NIST Webbook
tb	809.12	K	Joback Method
tc	992.99	K	Joback Method
tf	470.44	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.26	J/mol×K	809.12	Joback Method
cpg	957.88	J/mol×K	839.76	Joback Method
cpg	974.45	J/mol×K	870.41	Joback Method
cpg	989.99	J/mol×K	901.05	Joback Method
cpg	1004.48	J/mol×K	931.70	Joback Method
cpg	1017.95	J/mol×K	962.34	Joback Method
cpg	1030.39	J/mol×K	992.99	Joback Method
dvisc	0.0006407	Pa×s	470.44	Joback Method

dvisc	0.0003267	Pa×s	526.89	Joback Method
dvisc	0.0001897	Pa×s	583.33	Joback Method
dvisc	0.0001213	Pa×s	639.78	Joback Method
dvisc	0.0000834	Pa×s	696.23	Joback Method
dvisc	0.0000606	Pa×s	752.67	Joback Method
dvisc	0.0000461	Pa×s	809.12	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=U381863&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