Diglycolic acid, 3-methylpent-2-yl undecyl ester

Inchi: InChI=1S/C21H40O5/c1-5-7-8-9-10-11-12-13-14-15-25-20(22)16-24-17-21(23)26-19(4)1

InchiKey: OFINUMBULPYNJF-UHFFFAOYSA-N

Formula: C21H40O5

SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OC(C)C(C)CC

Mol. weight [g/mol]: 372.54

Physical Properties

Property code	Value	Unit	Source
gf	-451.78	kJ/mol	Joback Method
hf	-1109.15	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	5.055		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	3035.00		NIST Webbook
rinpol	3035.00		NIST Webbook
tb	854.00	K	Joback Method
tc	1046.11	K	Joback Method
tf	462.98	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.08	J/mol×K	854.00	Joback Method
cpg	1081.57	J/mol×K	886.02	Joback Method
cpg	1098.82	J/mol×K	918.04	Joback Method
cpg	1114.82	J/mol×K	950.06	Joback Method
cpg	1129.61	J/mol×K	982.07	Joback Method
cpg	1143.18	J/mol×K	1014.09	Joback Method
cpg	1155.54	J/mol×K	1046.11	Joback Method
dvisc	0.0006967	Pa×s	462.98	Joback Method

dvisc	0.0002952	Pa×s	528.15	Joback Method
dvisc	0.0001510	Pa×s	593.32	Joback Method
dvisc	0.0000882	Pa×s	658.49	Joback Method
dvisc	0.0000568	Pa×s	723.66	Joback Method
dvisc	0.0000393	Pa×s	788.83	Joback Method
dvisc	0.0000288	Pa×s	854.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381879&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

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