Diglycolic acid, 3,7-dimethyloctyl isohexyl ester

Inchi: InChI=1S/C20H38O5/c1-16(2)8-6-10-18(5)11-13-25-20(22)15-23-14-19(21)24-12-7-9-17

InchiKey: ZIYOCDSIMZRRNO-UHFFFAOYSA-N

Formula: C20H38O5

SMILES: CC(C)CCCOC(=O)COCC(=O)OCCC(C)CCCC(C)C

Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-462.64	kJ/mol	Joback Method
hf	-1093.79	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.378		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2830.00		NIST Webbook
tb	830.68	K	Joback Method
tc	1019.79	K	Joback Method
tf	436.71	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.28	J/mol×K	830.68	Joback Method
cpg	1020.47	J/mol×K	862.20	Joback Method
cpg	1037.49	J/mol×K	893.72	Joback Method
cpg	1053.34	J/mol×K	925.24	Joback Method
cpg	1068.02	J/mol×K	956.75	Joback Method
cpg	1081.56	J/mol×K	988.27	Joback Method
cpg	1093.95	J/mol×K	1019.79	Joback Method
dvisc	0.0009558	Pa×s	436.71	Joback Method
dvisc	0.0003706	Pa×s	502.37	Joback Method

dvisc	0.0001789	Pa×s	568.03	Joback Method
dvisc	0.0001004	Pa×s	633.69	Joback Method
dvisc	0.0000628	Pa×s	699.36	Joback Method
dvisc	0.0000426	Pa×s	765.02	Joback Method
dvisc	0.0000307	Pa×s	830.68	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=U382147&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