Diglycolic acid, 2-methylpentyl nonyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-466.18	kJ/mol	Joback Method
hf	-1062.59	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	808.68	K	Joback Method
tc	993.30	K	Joback Method
tf	455.44	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.75	J/mol×K	808.68	Joback Method
cpg	958.44	J/mol×K	839.45	Joback Method
cpg	975.07	J/mol×K	870.22	Joback Method
cpg	990.65	J/mol×K	900.99	Joback Method
cpg	1005.16	J/mol×K	931.76	Joback Method
cpg	1018.64	J/mol×K	962.53	Joback Method
cpg	1031.06	J/mol×K	993.30	Joback Method
dvisc	0.0007490	Pa×s	455.44	Joback Method

dvisc	0.0003527	Pa×s	514.31	Joback Method
dvisc	0.0001939	Pa×s	573.19	Joback Method
dvisc	0.0001192	Pa×s	632.06	Joback Method
dvisc	0.0000796	Pa×s	690.93	Joback Method
dvisc	0.0000566	Pa×s	749.81	Joback Method
dvisc	0.0000423	Pa×s	808.68	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=U381801&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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