Diglycolic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C20H38O5/c1-15(9-19(3,4)5)11-24-17(21)13-23-14-18(22)25-12-16(2)10-20(6
InchiKey: BGSIVQJXQZWKLE-UHFFFAOYSA-N
Formula: C20H38O5
SMILES: CC(COC(=O)COCC(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-454.52	kJ/mol	Joback Method
hf	-1106.01	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.234		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rinpol	2628.00		NIST Webbook
rinpol	2628.00		NIST Webbook
tb	824.66	K	Joback Method
tc	1018.35	K	Joback Method
tf	456.55	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.50	J/mol×K	824.66	Joback Method
cpg	1083.09	J/mol×K	986.07	Joback Method
cpg	1069.37	J/mol×K	953.79	Joback Method
cpg	1054.59	J/mol×K	921.50	Joback Method
cpg	1038.71	J/mol×K	889.22	Joback Method
cpg	1021.69	J/mol×K	856.94	Joback Method
cpg	1095.79	J/mol×K	1018.35	Joback Method
dvisc	0.0000212	Pa×s	824.66	Joback Method

dvisc	0.0000302	Pa×s	763.31	Joback Method
dvisc	0.0000456	Pa×s	701.96	Joback Method
dvisc	0.0000747	Pa×s	640.61	Joback Method
dvisc	0.0001356	Pa×s	579.25	Joback Method
dvisc	0.0002837	Pa×s	517.90	Joback Method
dvisc	0.0007238	Pa×s	456.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382053&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

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