Diglycolic acid, neopentyl undecyl ester

Inchi: InChI=1S/C20H38O5/c1-5-6-7-8-9-10-11-12-13-14-24-18(21)15-23-16-19(22)25-17-20(2
InchiKey: BQZVRQWNMHGHKA-UHFFFAOYSA-N
Formula: C20H38O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-452.48	kJ/mol	Joback Method
hf	-1086.70	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.666		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	828.77	K	Joback Method
tc	1017.43	K	Joback Method
tf	484.13	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.66	J/mol×K	828.77	Joback Method
cpg	1019.60	J/mol×K	860.21	Joback Method
cpg	1036.43	J/mol×K	891.66	Joback Method
cpg	1052.17	J/mol×K	923.10	Joback Method
cpg	1066.82	J/mol×K	954.55	Joback Method
cpg	1080.43	J/mol×K	985.99	Joback Method
cpg	1093.00	J/mol×K	1017.43	Joback Method
dvisc	0.0005354	Pa×s	484.13	Joback Method

dvisc	0.0002603	Pa×s	541.57	Joback Method
dvisc	0.0001453	Pa×s	599.01	Joback Method
dvisc	0.0000898	Pa×s	656.45	Joback Method
dvisc	0.0000600	Pa×s	713.89	Joback Method
dvisc	0.0000425	Pa×s	771.33	Joback Method
dvisc	0.0000316	Pa×s	828.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381923&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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