Diglycolic acid, dodecyl neopentyl ester

Inchi: InChI=1S/C21H40O5/c1-5-6-7-8-9-10-11-12-13-14-15-25-19(22)16-24-17-20(23)26-18-21(2
InchiKey: VNCPMPLZWOGOLO-UHFFFAOYSA-N
Formula: C21H40O5
SMILES: CCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 372.54

Physical Properties

Property code	Value	Unit	Source
gf	-444.06	kJ/mol	Joback Method
hf	-1107.34	kJ/mol	Joback Method
hfus	49.49	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.056		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	851.65	K	Joback Method
tc	1043.69	K	Joback Method
tf	495.40	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.72	J/mol×K	851.65	Joback Method
cpg	1081.03	J/mol×K	883.66	Joback Method
cpg	1098.15	J/mol×K	915.66	Joback Method
cpg	1114.10	J/mol×K	947.67	Joback Method
cpg	1128.92	J/mol×K	979.68	Joback Method
cpg	1142.62	J/mol×K	1011.68	Joback Method
cpg	1155.23	J/mol×K	1043.69	Joback Method
dvisc	0.0004724	Pa×s	495.40	Joback Method

dvisc	0.0002272	Pa×s	554.77	Joback Method
dvisc	0.0001259	Pa×s	614.15	Joback Method
dvisc	0.0000774	Pa×s	673.52	Joback Method
dvisc	0.0000515	Pa×s	732.90	Joback Method
dvisc	0.0000364	Pa×s	792.27	Joback Method
dvisc	0.0000271	Pa×s	851.65	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=U381924&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