Diglycolic acid, tridecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C25H48O5/c1-6-7-8-9-10-11-12-13-14-15-16-17-29-23(26)20-28-21-24(27)30-

InchiKey: WRTNHRNXYIIDRS-UHFFFAOYSA-N

Formula: C25H48O5

SMILES: CCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 428.65

Physical Properties

Property code	Value	Unit	Source
gf	-412.82	kJ/mol	Joback Method
hf	-1195.18	kJ/mol	Joback Method
hfus	56.33	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.473		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	808.91	kPa	Joback Method
rinpol	3411.00		NIST Webbook
rinpol	3411.00		NIST Webbook
tb	942.73	K	Joback Method
tc	1156.42	K	Joback Method
tf	525.48	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.44	J/mol×K	942.73	Joback Method
cpg	1333.33	J/mol×K	978.34	Joback Method
cpg	1351.63	J/mol×K	1013.96	Joback Method
cpg	1368.39	J/mol×K	1049.57	Joback Method
cpg	1383.66	J/mol×K	1085.19	Joback Method
cpg	1397.47	J/mol×K	1120.80	Joback Method
cpg	1409.89	J/mol×K	1156.42	Joback Method
dvisc	0.0003191	Pa×s	525.48	Joback Method

dvisc	0.0001370	Pa×s	595.02	Joback Method
dvisc	0.0000702	Pa×s	664.56	Joback Method
dvisc	0.0000408	Pa×s	734.11	Joback Method
dvisc	0.0000261	Pa×s	803.65	Joback Method
dvisc	0.0000179	Pa×s	873.19	Joback Method
dvisc	0.0000130	Pa×s	942.73	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=U382048&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

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