Acetic acid, [3-hydroxy-4,4'-carbonylbis(phenyleneoxy)di-], didodecyl ester

Inchi: InChI=1S/C41H62O8/c1-3-5-7-9-11-13-15-17-19-21-29-46-39(43)32-48-35-25-23-34(24-
InchiKey: JIVKFMXHZGNYIX-UHFFFAOYSA-N
Formula: C41H62O8
SMILES: CCCCCCCCCCCCOC(=O)COc1ccc(C(=O)c2ccc(OCC(=O)OCCCCCCCCCCCC)cc2O)c
Mol. weight [g/mol]: 682.93
CAS: 116436-40-9

Physical Properties

Property code	Value	Unit	Source
gf	-461.48	kJ/mol	Joback Method
hf	-1483.38	kJ/mol	Joback Method
hfus	104.58	kJ/mol	Joback Method
hvap	155.63	kJ/mol	Joback Method
log10ws	-11.83		Crippen Method
logp	10.309		Crippen Method
mcvol	575.090	ml/mol	McGowan Method
pc	553.11	kPa	Joback Method
tb	1532.71	K	Joback Method
tc	2172.05	K	Joback Method
tf	980.14	K	Joback Method
vc	2.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2184.16	J/mol×K	1532.71	Joback Method
cpg	2204.84	J/mol×K	1639.27	Joback Method
cpg	2223.29	J/mol×K	1745.82	Joback Method
cpg	2242.17	J/mol×K	1852.38	Joback Method
cpg	2264.12	J/mol×K	1958.94	Joback Method
cpg	2291.80	J/mol×K	2065.50	Joback Method
cpg	2327.84	J/mol×K	2172.05	Joback Method
dvisc	0.0000003	Pa×s	980.14	Joback Method
dvisc	0.0000001	Pa×s	1072.24	Joback Method

dvisc	7.6343551e-08	Pa×s	1164.33	Joback Method
dvisc	4.6501234e-08	Pa×s	1256.42	Joback Method
dvisc	3.0308525e-08	Pa×s	1348.52	Joback Method
dvisc	2.0865719e-08	Pa×s	1440.61	Joback Method
dvisc	1.5024004e-08	Pa×s	1532.71	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=C116436409&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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