Diethylmalonic acid, 5-methoxy-3-methylpentyl tridecyl ester

Inchi: InChI=1S/C27H52O5/c1-6-9-10-11-12-13-14-15-16-17-18-21-31-25(28)27(7-2,8-3)26(29)

InchiKey: DEGGHBKEFOHVRT-UHFFFAOYSA-N

Formula: C27H52O5

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 456.70

Physical Properties

Property code	Value	Unit	Source
gf	-395.98	kJ/mol	Joback Method
hf	-1236.46	kJ/mol	Joback Method
hfus	61.51	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	7.253		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	727.31	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	988.49	K	Joback Method
tc	1219.20	K	Joback Method
tf	548.02	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.38	J/mol×K	988.49	Joback Method
cpg	1462.25	J/mol×K	1026.94	Joback Method
cpg	1481.25	J/mol×K	1065.39	Joback Method
cpg	1498.43	J/mol×K	1103.85	Joback Method
cpg	1513.86	J/mol×K	1142.30	Joback Method
cpg	1527.61	J/mol×K	1180.75	Joback Method
cpg	1539.76	J/mol×K	1219.20	Joback Method
dvisc	0.0002391	Pa×s	548.02	Joback Method

dvisc	0.0001012	Pa×s	621.43	Joback Method
dvisc	0.0000513	Pa×s	694.84	Joback Method
dvisc	0.0000297	Pa×s	768.25	Joback Method
dvisc	0.0000189	Pa×s	841.67	Joback Method
dvisc	0.0000129	Pa×s	915.08	Joback Method
dvisc	0.0000093	Pa×s	988.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370772&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