Diethylmalonic acid, dodecyl pentadecyl ester

Inchi: InChI=1S/C34H66O4/c1-5-9-11-13-15-17-19-20-21-23-25-27-29-31-38-33(36)34(7-3,8-4)
InchiKey: DWQJENLLVDGXMW-UHFFFAOYSA-N
Formula: C34H66O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 538.89

Physical Properties

Property code	Value	Unit	Source
gf	-229.60	kJ/mol	Joback Method
hf	-1243.44	kJ/mol	Joback Method
hfus	81.98	kJ/mol	Joback Method
hvap	108.29	kJ/mol	Joback Method
log10ws	-11.54		Crippen Method
logp	10.891		Crippen Method
mcvol	504.800	ml/mol	McGowan Method
pc	523.41	kPa	Joback Method
rinpol	3424.00		NIST Webbook
rinpol	3424.00		NIST Webbook
tb	1126.67	K	Joback Method
tc	1450.76	K	Joback Method
tf	619.68	K	Joback Method
vc	1.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1869.38	J/mol×K	1126.67	Joback Method
cpg	1980.01	J/mol×K	1396.75	Joback Method
cpg	1962.94	J/mol×K	1342.73	Joback Method
cpg	1943.66	J/mol×K	1288.72	Joback Method
cpg	1921.85	J/mol×K	1234.70	Joback Method
cpg	1897.20	J/mol×K	1180.69	Joback Method
cpg	1995.20	J/mol×K	1450.76	Joback Method
dvisc	0.0000044	Pa×s	1126.67	Joback Method

dvisc	0.0000060	Pa×s	1042.17	Joback Method
dvisc	0.0000088	Pa×s	957.67	Joback Method
dvisc	0.0000139	Pa×s	873.17	Joback Method
dvisc	0.0000241	Pa×s	788.68	Joback Method
dvisc	0.0000476	Pa×s	704.18	Joback Method
dvisc	0.0001136	Pa×s	619.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369720&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

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