Diethylmalonic acid, 3,7-dimethyloctyl tridecyl ester

Inchi: InChI=1S/C30H58O4/c1-7-10-11-12-13-14-15-16-17-18-19-24-33-28(31)30(8-2,9-3)29(3

InchiKey: FCSIEMUHTKWWCI-UHFFFAOYSA-N

Formula: C30H58O4

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

Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-268.16	kJ/mol	Joback Method
hf	-1171.44	kJ/mol	Joback Method
hfus	64.57	kJ/mol	Joback Method
hvap	98.61	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	9.043		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	634.16	kPa	Joback Method
rinpol	2912.00		NIST Webbook
tb	1034.27	K	Joback Method
tc	1285.38	K	Joback Method
tf	544.60	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.20	J/mol×K	1034.27	Joback Method
cpg	1628.30	J/mol×K	1076.12	Joback Method
cpg	1649.33	J/mol×K	1117.97	Joback Method
cpg	1668.40	J/mol×K	1159.83	Joback Method
cpg	1685.65	J/mol×K	1201.68	Joback Method
cpg	1701.19	J/mol×K	1243.53	Joback Method
cpg	1715.17	J/mol×K	1285.38	Joback Method
dvisc	0.0002696	Pa×s	544.60	Joback Method
dvisc	0.0000990	Pa×s	626.21	Joback Method

dvisc	0.0000458	Pa×s	707.82	Joback Method
dvisc	0.0000248	Pa×s	789.43	Joback Method
dvisc	0.0000151	Pa×s	871.05	Joback Method
dvisc	0.0000100	Pa×s	952.66	Joback Method
dvisc	0.0000071	Pa×s	1034.27	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=U369412&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