Diethylmalonic acid, 3-methylpent-2-yl tridecyl ester

Inchi: InChI=1S/C26H50O4/c1-7-11-12-13-14-15-16-17-18-19-20-21-29-24(27)26(9-3,10-4)25(
InchiKey: DGSHXUWHNPZOOH-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-301.84	kJ/mol	Joback Method
hf	-1088.88	kJ/mol	Joback Method
hfus	54.21	kJ/mol	Joback Method
hvap	89.71	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.625		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	777.21	kPa	Joback Method
rinpol	2574.00		NIST Webbook
tb	942.75	K	Joback Method
tc	1155.89	K	Joback Method
tf	499.52	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.71	J/mol×K	942.75	Joback Method
cpg	1434.57	J/mol×K	1120.37	Joback Method
cpg	1419.57	J/mol×K	1084.85	Joback Method
cpg	1403.25	J/mol×K	1049.32	Joback Method
cpg	1385.54	J/mol×K	1013.80	Joback Method
cpg	1366.38	J/mol×K	978.27	Joback Method
cpg	1448.31	J/mol×K	1155.89	Joback Method
dvisc	0.0000138	Pa×s	942.75	Joback Method
dvisc	0.0000194	Pa×s	868.88	Joback Method

dvisc	0.0000292	Pa×s	795.01	Joback Method
dvisc	0.0000477	Pa×s	721.13	Joback Method
dvisc	0.0000872	Pa×s	647.26	Joback Method
dvisc	0.0001862	Pa×s	573.39	Joback Method
dvisc	0.0004975	Pa×s	499.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369738&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