Diethylmalonic acid, 2,4,4-trimethylpentyl undecyl ester

Inchi: InChI=1S/C26H50O4/c1-8-11-12-13-14-15-16-17-18-19-29-23(27)26(9-2,10-3)24(28)30-
InchiKey: SQGBMJRUOCXPNV-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-296.56	kJ/mol	Joback Method
hf	-1092.35	kJ/mol	Joback Method
hfus	50.32	kJ/mol	Joback Method
hvap	88.80	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.482		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	782.00	kPa	Joback Method
rinpol	2515.00		NIST Webbook
tb	939.96	K	Joback Method
tc	1151.35	K	Joback Method
tf	516.94	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.11	J/mol×K	939.96	Joback Method
cpg	1365.61	J/mol×K	975.19	Joback Method
cpg	1384.72	J/mol×K	1010.42	Joback Method
cpg	1402.52	J/mol×K	1045.65	Joback Method
cpg	1419.09	J/mol×K	1080.89	Joback Method
cpg	1434.53	J/mol×K	1116.12	Joback Method
cpg	1448.90	J/mol×K	1151.35	Joback Method
dvisc	0.0003817	Pa×s	516.94	Joback Method
dvisc	0.0001503	Pa×s	587.44	Joback Method

dvisc	0.0000723	Pa×s	657.95	Joback Method
dvisc	0.0000400	Pa×s	728.45	Joback Method
dvisc	0.0000246	Pa×s	798.95	Joback Method
dvisc	0.0000164	Pa×s	869.46	Joback Method
dvisc	0.0000116	Pa×s	939.96	Joback Method

Sources

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=U369483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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