Diethylmalonic acid, 2-isopropoxyphenyl tetradecyl ester

Inchi: InChI=1S/C30H50O5/c1-6-9-10-11-12-13-14-15-16-17-18-21-24-33-28(31)30(7-2,8-3)29

InchiKey: WDCULJIBPPWWLF-UHFFFAOYSA-N

Formula: C30H50O5

SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 490.71

Physical Properties

Property code	Value	Unit	Source
gf	-267.94	kJ/mol	Joback Method
hf	-1073.32	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	104.35	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.430		Crippen Method
mcvol	430.550	ml/mol	McGowan Method
pc	738.42	kPa	Joback Method
rinpol	3149.00		NIST Webbook
tb	1088.79	K	Joback Method
tc	1344.16	K	Joback Method
tf	620.77	K	Joback Method
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.07	J/mol×K	1088.79	Joback Method
cpg	1542.71	J/mol×K	1131.35	Joback Method
cpg	1558.26	J/mol×K	1173.91	Joback Method
cpg	1571.83	J/mol×K	1216.47	Joback Method
cpg	1583.51	J/mol×K	1259.04	Joback Method
cpg	1593.43	J/mol×K	1301.60	Joback Method
cpg	1601.69	J/mol×K	1344.16	Joback Method
dvisc	0.0001138	Pa×s	620.77	Joback Method
dvisc	0.0000530	Pa×s	698.77	Joback Method

dvisc	0.0000287	Pa×s	776.78	Joback Method
dvisc	0.0000174	Pa×s	854.78	Joback Method
dvisc	0.0000115	Pa×s	932.78	Joback Method
dvisc	0.0000081	Pa×s	1010.79	Joback Method
dvisc	0.0000060	Pa×s	1088.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369592&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