Diethylmalonic acid, 3-phenylpropyl tridecyl ester

Inchi: InChI=1S/C29H48O4/c1-4-7-8-9-10-11-12-13-14-15-19-24-32-27(30)29(5-2,6-3)28(31)33

InchiKey: OXJDZKGPIKIVGR-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-159.29	kJ/mol	Joback Method
hf	-903.71	kJ/mol	Joback Method
hfus	63.07	kJ/mol	Joback Method
hvap	99.44	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.823		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	789.04	kPa	Joback Method
rinpol	3112.00		NIST Webbook
rinpol	3112.00		NIST Webbook
tb	1038.95	K	Joback Method
tc	1276.31	K	Joback Method
tf	589.75	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.59	J/mol×K	1038.95	Joback Method
cpg	1452.33	J/mol×K	1078.51	Joback Method
cpg	1469.46	J/mol×K	1118.07	Joback Method
cpg	1485.09	J/mol×K	1157.63	Joback Method
cpg	1499.34	J/mol×K	1197.19	Joback Method
cpg	1512.31	J/mol×K	1236.75	Joback Method
cpg	1524.12	J/mol×K	1276.31	Joback Method
dvisc	0.0002030	Pa×s	589.75	Joback Method

dvisc	0.0000936	Pa×s	664.62	Joback Method
dvisc	0.0000505	Pa×s	739.48	Joback Method
dvisc	0.0000305	Pa×s	814.35	Joback Method
dvisc	0.0000201	Pa×s	889.22	Joback Method
dvisc	0.0000141	Pa×s	964.08	Joback Method
dvisc	0.0000104	Pa×s	1038.95	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=U369663&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

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