Diethylmalonic acid, nonyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C29H40O5/c1-4-7-8-9-10-11-15-21-32-27(30)29(5-2,6-3)28(31)33-23-24-17-16

InchiKey: HJCGIGCOJMICQJ-UHFFFAOYSA-N

Formula: C29H40O5

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-161.51	kJ/mol	Joback Method
hf	-810.87	kJ/mol	Joback Method
hfus	57.91	kJ/mol	Joback Method
hvap	104.79	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.622		Crippen Method
mcvol	392.700	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	3190.00		NIST Webbook
tb	1093.03	K	Joback Method
tc	1338.68	K	Joback Method
tf	650.92	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.99	J/mol×K	1093.03	Joback Method
cpg	1362.99	J/mol×K	1133.97	Joback Method
cpg	1375.31	J/mol×K	1174.91	Joback Method
cpg	1386.04	J/mol×K	1215.85	Joback Method
cpg	1395.30	J/mol×K	1256.79	Joback Method
cpg	1403.18	J/mol×K	1297.74	Joback Method
cpg	1409.79	J/mol×K	1338.68	Joback Method
dvisc	0.0001066	Pa×s	650.92	Joback Method
dvisc	0.0000557	Pa×s	724.61	Joback Method

dvisc	0.0000328	Pa×s	798.29	Joback Method
dvisc	0.0000211	Pa×s	871.98	Joback Method
dvisc	0.0000146	Pa×s	945.66	Joback Method
dvisc	0.0000106	Pa×s	1019.35	Joback Method
dvisc	0.0000081	Pa×s	1093.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370237&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

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