

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000328	Paxs	798.29	Joback Method
dvisc	0.0000211	Paxs	871.98	Joback Method
dvisc	0.0000146	Paxs	945.66	Joback Method
dvisc	0.0000106	Paxs	1019.35	Joback Method
dvisc	0.0000081	Paxs	1093.03	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=U370237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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