

Diethylmalonic acid, nonyl 3-phenylpropyl ester

Inchi:	InChI=1S/C25H40O4/c1-4-7-8-9-10-11-15-20-28-23(26)25(5-2,6-3)24(27)29-21-16-19-22
InchiKey:	YSTQNSIZYJRHPG-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-192.97	kJ/mol	Joback Method
hf	-821.15	kJ/mol	Joback Method
hfus	52.71	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.263		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinpol	2689.00		NIST Webbook
tb	947.43	K	Joback Method
tc	1160.67	K	Joback Method
tf	544.67	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.88	J/molxK	947.43	Joback Method
cpg	1199.24	J/molxK	982.97	Joback Method
cpg	1215.27	J/molxK	1018.51	Joback Method
cpg	1230.05	J/molxK	1054.05	Joback Method
cpg	1243.64	J/molxK	1089.59	Joback Method
cpg	1256.11	J/molxK	1125.13	Joback Method
cpg	1267.53	J/molxK	1160.67	Joback Method
dvisc	0.0003495	Paxs	544.67	Joback Method
dvisc	0.0001667	Paxs	611.80	Joback Method

dvisc	0.0000920	Paxs	678.92	Joback Method
dvisc	0.0000566	Paxs	746.05	Joback Method
dvisc	0.0000377	Paxs	813.18	Joback Method
dvisc	0.0000267	Paxs	880.30	Joback Method
dvisc	0.0000199	Paxs	947.43	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=U369659&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

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