

Diethylmalonic acid, nonyl phenethyl ester

Inchi:	InChI=1S/C24H38O4/c1-4-7-8-9-10-11-15-19-27-22(25)24(5-2,6-3)23(26)28-20-18-21-16
InchiKey:	DAFVTGAVZWJLZ-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-201.39	kJ/mol	Joback Method
hf	-800.51	kJ/mol	Joback Method
hfus	50.12	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.872		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinsol	2537.00		NIST Webbook
tb	924.55	K	Joback Method
tc	1134.34	K	Joback Method
tf	533.40	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.14	J/molxK	924.55	Joback Method
cpg	1193.58	J/molxK	1099.37	Joback Method
cpg	1181.20	J/molxK	1064.41	Joback Method
cpg	1167.73	J/molxK	1029.44	Joback Method
cpg	1153.10	J/molxK	994.48	Joback Method
cpg	1137.26	J/molxK	959.51	Joback Method
cpg	1204.94	J/molxK	1134.34	Joback Method
dvisc	0.0000232	Paxs	924.55	Joback Method
dvisc	0.0000312	Paxs	859.36	Joback Method

dvisc	0.0000439	Paxs	794.17	Joback Method
dvisc	0.0000657	Paxs	728.97	Joback Method
dvisc	0.0001064	Paxs	663.78	Joback Method
dvisc	0.0001915	Paxs	598.59	Joback Method
dvisc	0.0003979	Paxs	533.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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