

Diethylmalonic acid, nonyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C24H46O4/c1-8-11-12-13-14-15-16-17-27-21(25)24(9-2,10-3)22(26)28-19-20(
InchiKey:	YCRWRGMLGWJWCB-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-313.40	kJ/mol	Joback Method
hf	-1051.07	kJ/mol	Joback Method
hfus	45.14	kJ/mol	Joback Method
hvap	84.35	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.702		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinsol	2313.00		NIST Webbook
tb	894.20	K	Joback Method
tc	1095.17	K	Joback Method
tf	494.40	K	Joback Method
vc	1.399	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.18	J/molxK	894.20	Joback Method
cpg	1237.82	J/molxK	927.69	Joback Method
cpg	1256.21	J/molxK	961.19	Joback Method
cpg	1273.40	J/molxK	994.68	Joback Method
cpg	1289.46	J/molxK	1028.18	Joback Method
cpg	1304.45	J/molxK	1061.67	Joback Method
cpg	1318.45	J/molxK	1095.17	Joback Method
dvisc	0.0005168	Paxs	494.40	Joback Method
dvisc	0.0002062	Paxs	561.03	Joback Method

dvisc	0.0001000	Paxs	627.67	Joback Method
dvisc	0.0000557	Paxs	694.30	Joback Method
dvisc	0.0000344	Paxs	760.93	Joback Method
dvisc	0.0000229	Paxs	827.57	Joback Method
dvisc	0.0000162	Paxs	894.20	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=U369481&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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