

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

Inchi:	InChI=1S/C27H52O4/c1-8-11-12-13-14-15-16-17-18-19-20-30-24(28)27(9-2,10-3)25(29)
InchiKey:	JHZBZSZBPGZVLX-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-288.14	kJ/mol	Joback Method
hf	-1112.99	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	91.03	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.872		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	741.64	kPa	Joback Method
rinpol	2614.00		NIST Webbook
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tb	962.84	K	Joback Method
tc	1181.00	K	Joback Method
tf	528.21	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.34	J/molxK	962.84	Joback Method
cpg	1500.64	J/molxK	1144.64	Joback Method
cpg	1484.94	J/molxK	1108.28	Joback Method
cpg	1468.06	J/molxK	1071.92	Joback Method
cpg	1449.89	J/molxK	1035.56	Joback Method
cpg	1430.35	J/molxK	999.20	Joback Method
cpg	1515.24	J/molxK	1181.00	Joback Method
dvisc	0.0000098	Paxs	962.84	Joback Method

dvisc	0.0000138	Paxs	890.40	Joback Method
dvisc	0.0000208	Paxs	817.96	Joback Method
dvisc	0.0000339	Paxs	745.52	Joback Method
dvisc	0.0000613	Paxs	673.09	Joback Method
dvisc	0.0001281	Paxs	600.65	Joback Method
dvisc	0.0003272	Paxs	528.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369484&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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