

Diethylmalonic acid, dodecyl undecyl ester

Inchi:	InChI=1S/C30H58O4/c1-5-9-11-13-15-17-19-21-23-25-27-34-29(32)30(7-3,8-4)28(31)33
InchiKey:	MDXPFHRRQOLCHT-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-263.28	kJ/mol	Joback Method
hf	-1160.88	kJ/mol	Joback Method
hfus	71.62	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	9.331		Crippen Method
mvol	448.440	ml/mol	McGowan Method
pc	629.08	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	1035.15	K	Joback Method
tc	1291.99	K	Joback Method
tf	574.60	K	Joback Method
vc	1.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.78	J/molxK	1035.15	Joback Method
cpg	1628.56	J/molxK	1077.96	Joback Method
cpg	1650.20	J/molxK	1120.76	Joback Method
cpg	1669.84	J/molxK	1163.57	Joback Method
cpg	1687.63	J/molxK	1206.38	Joback Method
cpg	1703.68	J/molxK	1249.18	Joback Method
cpg	1718.15	J/molxK	1291.99	Joback Method
dvisc	0.0002068	Paxs	574.60	Joback Method

dvisc	0.0000890	Paxs	651.36	Joback Method
dvisc	0.0000457	Paxs	728.12	Joback Method
dvisc	0.0000267	Paxs	804.88	Joback Method
dvisc	0.0000171	Paxs	881.63	Joback Method
dvisc	0.0000118	Paxs	958.39	Joback Method
dvisc	0.0000086	Paxs	1035.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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