

Diethylmalonic acid, dodecyl pentyl ester

Inchi:	InChI=1S/C24H46O4/c1-5-9-11-12-13-14-15-16-17-19-21-28-23(26)24(7-3,8-4)22(25)27
InchiKey:	FLLLMXIHGGMJBW-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-313.80	kJ/mol	Joback Method
hf	-1037.04	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	86.03	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.990		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	2459.00		NIST Webbook
tb	897.87	K	Joback Method
tc	1099.42	K	Joback Method
tf	506.98	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.64	J/molxK	897.87	Joback Method
cpg	1237.51	J/molxK	931.46	Joback Method
cpg	1256.06	J/molxK	965.05	Joback Method
cpg	1273.35	J/molxK	998.65	Joback Method
cpg	1289.41	J/molxK	1032.24	Joback Method
cpg	1304.32	J/molxK	1065.83	Joback Method
cpg	1318.10	J/molxK	1099.42	Joback Method
dvisc	0.0004804	Paxs	506.98	Joback Method
dvisc	0.0002166	Paxs	572.13	Joback Method

dvisc	0.0001149	Paxs	637.28	Joback Method
dvisc	0.0000686	Paxs	702.42	Joback Method
dvisc	0.0000447	Paxs	767.57	Joback Method
dvisc	0.0000311	Paxs	832.72	Joback Method
dvisc	0.0000228	Paxs	897.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369715&Units=SI

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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