

Diethylmalonic acid, 5-methoxy-3-methylpentyl undecyl ester

Inchi:	InChI=1S/C25H48O5/c1-6-9-10-11-12-13-14-15-16-19-29-23(26)25(7-2,8-3)24(27)30-21
InchiKey:	RCJRVRXQZHKQCX-UHFFFAOYSA-N
Formula:	C25H48O5
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	428.65

Physical Properties

Property code	Value	Unit	Source
gf	-412.82	kJ/mol	Joback Method
hf	-1195.18	kJ/mol	Joback Method
hfus	56.33	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.473		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	808.91	kPa	Joback Method
rinpol	2606.00		NIST Webbook
tb	942.73	K	Joback Method
tc	1156.42	K	Joback Method
tf	525.48	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.44	J/molxK	942.73	Joback Method
cpg	1397.47	J/molxK	1120.80	Joback Method
cpg	1383.66	J/molxK	1085.19	Joback Method
cpg	1368.39	J/molxK	1049.57	Joback Method
cpg	1351.63	J/molxK	1013.96	Joback Method
cpg	1333.33	J/molxK	978.34	Joback Method
cpg	1409.89	J/molxK	1156.42	Joback Method
dvisc	0.0000130	Paxs	942.73	Joback Method
dvisc	0.0000179	Paxs	873.19	Joback Method

dvisc	0.0000261	Paxs	803.65	Joback Method
dvisc	0.0000408	Paxs	734.11	Joback Method
dvisc	0.0000702	Paxs	664.56	Joback Method
dvisc	0.0001370	Paxs	595.02	Joback Method
dvisc	0.0003191	Paxs	525.48	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=U370770&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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