

Diethylmalonic acid, 2-ethoxyethyl tridecyl ester

Inchi:	InChI=1S/C24H46O5/c1-5-9-10-11-12-13-14-15-16-17-18-19-28-22(25)24(6-2,7-3)23(26)
InchiKey:	ZLVMHBUXWRNDBJ-UHFFFAOYSA-N
Formula:	C24H46O5
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	414.62

Physical Properties

Property code	Value	Unit	Source
gf	-418.80	kJ/mol	Joback Method
hf	-1169.26	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	88.44	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	6.227		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	920.29	K	Joback Method
tc	1127.80	K	Joback Method
tf	529.21	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.68	J/molxK	920.29	Joback Method
cpg	1269.22	J/molxK	954.87	Joback Method
cpg	1287.30	J/molxK	989.46	Joback Method
cpg	1303.94	J/molxK	1024.04	Joback Method
cpg	1319.19	J/molxK	1058.63	Joback Method
cpg	1333.10	J/molxK	1093.21	Joback Method
cpg	1345.71	J/molxK	1127.80	Joback Method
dvisc	0.0003189	Paxs	529.21	Joback Method

dvisc	0.0001491	Paxs	594.39	Joback Method
dvisc	0.0000810	Paxs	659.57	Joback Method
dvisc	0.0000491	Paxs	724.75	Joback Method
dvisc	0.0000323	Paxs	789.93	Joback Method
dvisc	0.0000227	Paxs	855.11	Joback Method
dvisc	0.0000167	Paxs	920.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370614&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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