

Diethylmalonic acid, 2-ethoxyethyl hexadecyl ester

Inchi:	InChI=1S/C27H52O5/c1-5-9-10-11-12-13-14-15-16-17-18-19-20-21-22-31-25(28)27(6-2,
InchiKey:	WNFNBNZNFVLES-UHFFFAOYSA-N
Formula:	C27H52O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	456.70

Physical Properties

Property code	Value	Unit	Source
gf	-393.54	kJ/mol	Joback Method
hf	-1231.18	kJ/mol	Joback Method
hfus	65.03	kJ/mol	Joback Method
hvap	95.12	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.397		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	724.18	kPa	Joback Method
rinpol	2837.00		NIST Webbook
tb	988.93	K	Joback Method
tc	1221.53	K	Joback Method
tf	563.02	K	Joback Method
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.07	J/molxK	988.93	Joback Method
cpg	1462.16	J/molxK	1027.70	Joback Method
cpg	1481.36	J/molxK	1066.46	Joback Method
cpg	1498.74	J/molxK	1105.23	Joback Method
cpg	1514.35	J/molxK	1144.00	Joback Method
cpg	1528.27	J/molxK	1182.77	Joback Method
cpg	1540.58	J/molxK	1221.53	Joback Method
dvisc	0.0002106	Paxs	563.02	Joback Method
dvisc	0.0000960	Paxs	634.00	Joback Method

dvisc	0.0000512	Paxs	704.99	Joback Method
dvisc	0.0000307	Paxs	775.97	Joback Method
dvisc	0.0000200	Paxs	846.96	Joback Method
dvisc	0.0000140	Paxs	917.94	Joback Method
dvisc	0.0000102	Paxs	988.93	Joback Method

Sources

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=U370617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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