

Diethylmalonic acid, di(2-methoxyethyl) ester

Inchi:	InChI=1S/C13H24O6/c1-5-13(6-2,11(14)18-9-7-16-3)12(15)19-10-8-17-4/h5-10H2,1-4H3
InchiKey:	GTGKJDYHUJAMQT-UHFFFAOYSA-N
Formula:	C13H24O6
SMILES:	CCC(CC)(C(=O)OCCOC)C(=O)OCCOC
Mol. weight [g/mol]:	276.33

Physical Properties

Property code	Value	Unit	Source
gf	-616.42	kJ/mol	Joback Method
hf	-1074.44	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	1.172		Crippen Method
mcvol	220.650	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1620.00		NIST Webbook
tb	691.03	K	Joback Method
tc	874.39	K	Joback Method
tf	427.47	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.24	J/molxK	691.03	Joback Method
cpg	642.37	J/molxK	721.59	Joback Method
cpg	656.72	J/molxK	752.15	Joback Method
cpg	670.27	J/molxK	782.71	Joback Method
cpg	683.03	J/molxK	813.27	Joback Method
cpg	694.99	J/molxK	843.83	Joback Method
cpg	706.15	J/molxK	874.39	Joback Method
dvisc	0.0007922	Paxs	427.47	Joback Method
dvisc	0.0004345	Paxs	471.40	Joback Method

dvisc	0.0002640	Paxs	515.32	Joback Method
dvisc	0.0001734	Paxs	559.25	Joback Method
dvisc	0.0001211	Paxs	603.18	Joback Method
dvisc	0.0000888	Paxs	647.10	Joback Method
dvisc	0.0000678	Paxs	691.03	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=U370685&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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