

Diethylmalonic acid, heptyl 2-methoxyethyl ester

Inchi:	InChI=1S/C17H32O5/c1-5-8-9-10-11-12-21-15(18)17(6-2,7-3)16(19)22-14-13-20-4/h5-14
InchiKey:	ZAXZKKMLSYTMIW-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOC
Mol. weight [g/mol]:	316.43

Physical Properties

Property code	Value	Unit	Source
gf	-477.74	kJ/mol	Joback Method
hf	-1024.78	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.496		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	1899.00		NIST Webbook
tb	760.13	K	Joback Method
tc	943.10	K	Joback Method
tf	450.32	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.20	J/molxK	760.13	Joback Method
cpg	898.46	J/molxK	912.61	Joback Method
cpg	885.25	J/molxK	882.11	Joback Method
cpg	871.14	J/molxK	851.62	Joback Method
cpg	856.10	J/molxK	821.12	Joback Method
cpg	840.12	J/molxK	790.63	Joback Method
cpg	910.76	J/molxK	943.10	Joback Method
dvisc	0.0000501	Paxs	760.13	Joback Method
dvisc	0.0000669	Paxs	708.50	Joback Method

dvisc	0.0000934	Paxs	656.86	Joback Method
dvisc	0.0001380	Paxs	605.23	Joback Method
dvisc	0.0002195	Paxs	553.59	Joback Method
dvisc	0.0003841	Paxs	501.96	Joback Method
dvisc	0.0007640	Paxs	450.32	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=U370675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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