

Diethylmalonic acid, 4-methoxyphenyl pentyl ester

Inchi:	InChI=1S/C19H28O5/c1-5-8-9-14-23-17(20)19(6-2,7-3)18(21)24-16-12-10-15(22-4)11-13
InchiKey:	HYJLDSHQDNONFY-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-358.12	kJ/mol	Joback Method
hf	-841.00	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.140		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinsol	2278.00		NIST Webbook
tb	837.55	K	Joback Method
tc	1043.24	K	Joback Method
tf	511.80	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.26	J/molxK	837.55	Joback Method
cpg	864.87	J/molxK	871.83	Joback Method
cpg	879.30	J/molxK	906.11	Joback Method
cpg	892.58	J/molxK	940.40	Joback Method
cpg	904.73	J/molxK	974.68	Joback Method
cpg	915.78	J/molxK	1008.96	Joback Method
cpg	925.75	J/molxK	1043.24	Joback Method
dvisc	0.0004207	Paxs	511.80	Joback Method
dvisc	0.0002318	Paxs	566.09	Joback Method

dvisc	0.0001418	Paxs	620.38	Joback Method
dvisc	0.0000938	Paxs	674.67	Joback Method
dvisc	0.0000660	Paxs	728.97	Joback Method
dvisc	0.0000488	Paxs	783.26	Joback Method
dvisc	0.0000375	Paxs	837.55	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=U369840&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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