

4-Pentenoic acid, 2,3-diethoxy-5-phenyl, ethyl ester

Inchi:	InChI=1S/C17H24O4/c1-4-19-15(13-12-14-10-8-7-9-11-14)16(20-5-2)17(18)21-6-3/h7-13
InchiKey:	KNOZDRZJNABUIT-OUKQBFOZSA-N
Formula:	C17H24O4
SMILES:	CCOC(=O)C(OCC)C(C=Cc1ccccc1)OCC
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-163.91	kJ/mol	Joback Method
hf	-560.26	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.073		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	739.45	K	Joback Method
tc	943.21	K	Joback Method
tf	389.31	K	Joback Method
vc	0.907	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.66	J/molxK	739.45	Joback Method
cpg	707.41	J/molxK	773.41	Joback Method
cpg	723.09	J/molxK	807.37	Joback Method
cpg	737.73	J/molxK	841.33	Joback Method
cpg	751.34	J/molxK	875.29	Joback Method
cpg	763.94	J/molxK	909.25	Joback Method
cpg	775.57	J/molxK	943.21	Joback Method
dvisc	0.0011221	Paxs	389.31	Joback Method

dvisc	0.0004684	Paxs	447.67	Joback Method
dvisc	0.0002392	Paxs	506.02	Joback Method
dvisc	0.0001404	Paxs	564.38	Joback Method
dvisc	0.0000910	Paxs	622.74	Joback Method
dvisc	0.0000636	Paxs	681.09	Joback Method
dvisc	0.0000470	Paxs	739.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329456&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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