

Propanoic acid, 2,3-diethoxy-3-phenyl, ethyl ester, threo

Inchi:	InChI=1S/C15H22O4/c1-4-17-13(12-10-8-7-9-11-12)14(18-5-2)15(16)19-6-3/h7-11,13-14
InchiKey:	DNGYVICCFRGRKH-UONOGXRCSA-N
Formula:	C15H22O4
SMILES:	CCOC(=O)C(OCC)C(OCC)c1ccccc1
Mol. weight [g/mol]:	266.33

Physical Properties

Property code	Value	Unit	Source
gf	-260.97	kJ/mol	Joback Method
hf	-636.20	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	64.46	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.732		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinsol	1584.00		NIST Webbook
tb	689.53	K	Joback Method
tc	890.91	K	Joback Method
tf	371.85	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.48	J/molxK	689.53	Joback Method
cpg	620.14	J/molxK	723.09	Joback Method
cpg	635.81	J/molxK	756.66	Joback Method
cpg	650.49	J/molxK	790.22	Joback Method
cpg	664.20	J/molxK	823.79	Joback Method
cpg	676.93	J/molxK	857.35	Joback Method
cpg	688.69	J/molxK	890.91	Joback Method
dvisc	0.0014594	Paxs	371.85	Joback Method
dvisc	0.0006432	Paxs	424.80	Joback Method

dvisc	0.0003399	Paxs	477.74	Joback Method
dvisc	0.0002040	Paxs	530.69	Joback Method
dvisc	0.0001343	Paxs	583.64	Joback Method
dvisc	0.0000948	Paxs	636.58	Joback Method
dvisc	0.0000706	Paxs	689.53	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=R329510&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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