

3,4,5-Triethoxybenzoic acid

Other names:	Benzoic acid, 3,4,5-triethoxy-
Inchi:	InChI=1S/C13H18O5/c1-4-16-10-7-9(13(14)15)8-11(17-5-2)12(10)18-6-3/h7-8H,4-6H2,1
InchiKey:	YCENSLDYFDZUMO-UHFFFAOYSA-N
Formula:	C13H18O5
SMILES:	CCOc1cc(C(=O)O)cc(OCC)c1OCC
Mol. weight [g/mol]:	254.28
CAS:	6970-19-0

Physical Properties

Property code	Value	Unit	Source
gf	-438.64	kJ/mol	Joback Method
hf	-771.00	kJ/mol	Joback Method
hfus	31.55	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.581		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	751.77	K	Joback Method
tc	945.53	K	Joback Method
tf	477.69	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.95	J/molxK	751.77	Joback Method
cpg	604.76	J/molxK	913.24	Joback Method
cpg	595.53	J/molxK	880.94	Joback Method
cpg	585.53	J/molxK	848.65	Joback Method
cpg	574.75	J/molxK	816.36	Joback Method
cpg	563.22	J/molxK	784.06	Joback Method
cpg	613.18	J/molxK	945.53	Joback Method
dvisc	0.0000213	Paxs	751.77	Joback Method

dvisc	0.0000294	Paxs	706.09	Joback Method
dvisc	0.0000425	Paxs	660.41	Joback Method
dvisc	0.0000648	Paxs	614.73	Joback Method
dvisc	0.0001057	Paxs	569.05	Joback Method
dvisc	0.0001877	Paxs	523.37	Joback Method
dvisc	0.0003722	Paxs	477.69	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=C6970190&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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