

Benzoic acid 5-ethoxy-4-methoxy-2-methoxymethyl-tetrahydro-

Inchi:
ester

InChI=1S/C17H24O6/c1-4-22-16-9-14(12(10-19-2)8-15(16)20-3)17(18)23-13-6-5-7-21-1

InchiKey:

OHNJATDBEBQAOB-UHFFFAOYSA-N

Formula:

C17H24O6

SMILES:

CCOc1cc(C(=O)OC2CCOC2)c(COC)cc1OC

Mol. weight [g/mol]:

324.37

Physical Properties

Property code	Value	Unit	Source
gf	-434.81	kJ/mol	Joback Method
hf	-911.23	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.576		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2135.14		NIST Webbook
rinpol	2096.31		NIST Webbook
rinpol	2096.31		NIST Webbook
tb	820.03	K	Joback Method
tc	1037.10	K	Joback Method
tf	518.13	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.63	J/molxK	820.03	Joback Method
cpg	785.18	J/molxK	856.21	Joback Method
cpg	800.27	J/molxK	892.39	Joback Method
cpg	813.89	J/molxK	928.57	Joback Method
cpg	826.00	J/molxK	964.75	Joback Method
cpg	836.59	J/molxK	1000.93	Joback Method
cpg	845.63	J/molxK	1037.10	Joback Method

dvisc	0.0003466	Paxs	518.13	Joback Method
dvisc	0.0002120	Paxs	568.45	Joback Method
dvisc	0.0001405	Paxs	618.76	Joback Method
dvisc	0.0000990	Paxs	669.08	Joback Method
dvisc	0.0000733	Paxs	719.40	Joback Method
dvisc	0.0000565	Paxs	769.71	Joback Method
dvisc	0.0000449	Paxs	820.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273764&Units=SI
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

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
mccvol:	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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