Benzoic acid 5-ethoxy-2-ethoxymethyl-4-methoxy-tetrahydro-py ester

Inchi: InChI=1S/C18H26O6/c1-4-21-11-13-9-16(20-3)17(23-5-2)10-15(13)18(19)24-14-7-6-8-22
InchiKey: OYCOANLWWRNLER-UHFFFAOYSA-N
Formula: C18H26O6
SMILES: CCOCc1cc(OC)c(OCC)cc1C(=O)OC1CCCOC1
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-426.39	kJ/mol	Joback Method
hf	-931.87	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.966		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2143.20		NIST Webbook
rinpol	2180.69		NIST Webbook
rinpol	2143.20		NIST Webbook
tb	842.91	K	Joback Method
tc	1058.34	K	Joback Method
tf	529.40	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.91	J/mol×K	842.91	Joback Method
cpg	843.42	J/mol×K	878.82	Joback Method
cpg	858.43	J/mol×K	914.72	Joback Method
cpg	871.92	J/mol×K	950.63	Joback Method
cpg	883.86	J/mol×K	986.53	Joback Method
cpg	894.23	J/mol×K	1022.44	Joback Method
cpg	903.02	J/mol×K	1058.34	Joback Method

dvisc	0.0003145	Pa×s	529.40	Joback Method
dvisc	0.0001900	Pa×s	581.65	Joback Method
dvisc	0.0001247	Pa×s	633.90	Joback Method
dvisc	0.0000873	Pa×s	686.15	Joback Method
dvisc	0.0000643	Pa×s	738.41	Joback Method
dvisc	0.0000493	Pa×s	790.66	Joback Method
dvisc	0.0000390	Pa×s	842.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R273759&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