ethyl [4,4,6,6,6-2H5]-5-benzyloxy-3-hydroxy-3-methylpe

Inchi: InChI=1S/C15H22O4/c1-3-19-14(16)11-15(2,17)9-10-18-12-13-7-5-4-6-8-13/h4-8,17H,3,

InchiKey: JWHXOHDFTSUPNZ-OXSMHHRZSA-N

Formula: C15H17D5O4

SMILES: CCOC(=O)CC(C)(O)CCOCc1ccccc1

Mol. weight [g/mol]: 271.36

Physical Properties

Property code	Value	Unit	Source
gf	-285.07	kJ/mol	Joback Method
hf	-654.40	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	78.21	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.297		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	756.94	K	Joback Method
tc	953.72	K	Joback Method
tf	442.86	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.32	J/mol×K	756.94	Joback Method
cpg	652.13	J/mol×K	789.74	Joback Method
cpg	665.04	J/mol×K	822.53	Joback Method
cpg	677.09	J/mol×K	855.33	Joback Method
cpg	688.32	J/mol×K	888.13	Joback Method
cpg	698.75	J/mol×K	920.92	Joback Method
cpg	708.42	J/mol×K	953.72	Joback Method
dvisc	0.0008928	Pa×s	442.86	Joback Method

dvisc	0.0003271	Pa×s	495.21	Joback Method
dvisc	0.0001452	Pa×s	547.55	Joback Method
dvisc	0.0000743	Pa×s	599.90	Joback Method
dvisc	0.0000423	Pa×s	652.25	Joback Method
dvisc	0.0000262	Pa×s	704.59	Joback Method
dvisc	0.0000173	Pa×s	756.94	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=R412414&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume