[1,1,1-2H3]-4-Benzyloxy-2-butanol

Inchi: InChI=1S/C11H16O2/c1-10(12)7-8-13-9-11-5-3-2-4-6-11/h2-6,10,12H,7-9H2,1H3/i1D3
InchiKey: PPVYBGKNKMMISH-FIBGUPNXSA-N
Formula: C11H13D3O2
SMILES: CC(O)CCOCc1ccccc1
Mol. weight [g/mol]: 183.26

Physical Properties

Property code	Value	Unit	Source
gf	-90.11	kJ/mol	Joback Method
hf	-323.57	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	61.06	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.974		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	591.92	K	Joback Method
tc	784.25	K	Joback Method
tf	308.20	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.96	J/mol×K	591.92	Joback Method
cpg	397.25	J/mol×K	623.98	Joback Method
cpg	409.84	J/mol×K	656.03	Joback Method
cpg	421.75	J/mol×K	688.09	Joback Method
cpg	433.00	J/mol×K	720.14	Joback Method
cpg	443.60	J/mol×K	752.20	Joback Method
cpg	453.58	J/mol×K	784.25	Joback Method
dvisc	0.0100219	Pa×s	308.20	Joback Method

dvisc	0.0024550	Pa×s	355.49	Joback Method
dvisc	0.0008368	Pa×s	402.77	Joback Method
dvisc	0.0003576	Pa×s	450.06	Joback Method
dvisc	0.0001796	Pa×s	497.35	Joback Method
dvisc	0.0001017	Pa×s	544.63	Joback Method
dvisc	0.0000630	Pa×s	591.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412385&Units=SI
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

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