

Bibenzyl, «alpha»,«alpha»'-epoxy-, cis-

Inchi:	InChI=1S/C14H12O/c1-3-7-11(8-4-1)13-14(15-13)12-9-5-2-6-10-12/h1-10,13-14H/t13-,14
InchiKey:	ARCJQKUWGAZPFX-OKILXGFUSA-N
Formula:	C14H12O
SMILES:	c1ccc(C2OC2c2ccccc2)cc1
Mol. weight [g/mol]:	196.24
CAS:	1689-71-0

Physical Properties

Property code	Value	Unit	Source
gf	258.74	kJ/mol	Joback Method
hf	61.23	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
ie	8.68	eV	NIST Webbook
log10ws	-3.79		Crippen Method
logp	3.499		Crippen Method
mcvol	155.610	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	602.10	K	Joback Method
tc	856.76	K	Joback Method
tf	340.65	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.41	J/molxK	602.10	Joback Method
cpg	408.45	J/molxK	644.54	Joback Method
cpg	424.95	J/molxK	686.99	Joback Method
cpg	440.01	J/molxK	729.43	Joback Method
cpg	453.76	J/molxK	771.87	Joback Method
cpg	466.33	J/molxK	814.32	Joback Method
cpg	477.83	J/molxK	856.76	Joback Method
dvisc	0.0020960	Paxs	340.65	Joback Method

dvisc	0.0014251	Paxs	384.23	Joback Method
dvisc	0.0010481	Paxs	427.80	Joback Method
dvisc	0.0008160	Paxs	471.38	Joback Method
dvisc	0.0006627	Paxs	514.95	Joback Method
dvisc	0.0005560	Paxs	558.52	Joback Method
dvisc	0.0004785	Paxs	602.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C1689710&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
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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