4-Benzyloxybenzoic acid

Other names: Benzoic acid, 4-(phenylmethoxy)-
p-(benzyloxy)benzoic acid
Inchi: InChI=1S/C14H12O3/c15-14(16)12-6-8-13(9-7-12)17-10-11-4-2-1-3-5-11/h1-9H,10H2,(H
InchiKey: AQSCHALQLXXKKC-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: O=C(O)c1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 228.24
CAS: 1486-51-7

Physical Properties

Property code	Value	Unit	Source
gf	-88.55	kJ/mol	Joback Method
hf	-267.73	kJ/mol	Joback Method
hfus	26.58	kJ/mol	Joback Method
hvap	77.81	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.964		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	746.53	K	Joback Method
tc	970.42	K	Joback Method
tf	445.88	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.37	J/mol×K	746.53	Joback Method
cpg	477.06	J/mol×K	783.85	Joback Method
cpg	487.82	J/mol×K	821.16	Joback Method
cpg	497.68	J/mol×K	858.48	Joback Method
cpg	506.70	J/mol×K	895.79	Joback Method
cpg	514.90	J/mol×K	933.11	Joback Method
cpg	522.33	J/mol×K	970.42	Joback Method

dvisc	0.0009347	Pa×s	445.88	Joback Method
dvisc	0.0004012	Pa×s	495.99	Joback Method
dvisc	0.0002012	Pa×s	546.10	Joback Method
dvisc	0.0001133	Pa×s	596.20	Joback Method
dvisc	0.0000697	Pa×s	646.31	Joback Method
dvisc	0.0000460	Pa×s	696.42	Joback Method
dvisc	0.0000321	Pa×s	746.53	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=C1486517&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume