

4-Bromodesoxybenzoin

Other names:	Benzyl 4-bromophenyl ketone Ethanone, 1-(4-bromophenyl)-2-phenyl-
Inchi:	InChI=1S/C14H11BrO/c15-13-8-6-12(7-9-13)14(16)10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	MOSIKPSTRPODHQ-UHFFFAOYSA-N
Formula:	C14H11BrO
SMILES:	O=C(Cc1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]:	275.14
CAS:	2001-29-8

Physical Properties

Property code	Value	Unit	Source
gf	167.59	kJ/mol	Joback Method
hf	43.05	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.874		Crippen Method
mcvol	179.670	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	698.09	K	Joback Method
tc	957.04	K	Joback Method
tf	422.63	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.04	J/molxK	698.09	Joback Method
cpg	439.70	J/molxK	741.25	Joback Method
cpg	452.15	J/molxK	784.41	Joback Method
cpg	463.48	J/molxK	827.56	Joback Method
cpg	473.80	J/molxK	870.72	Joback Method
cpg	483.20	J/molxK	913.88	Joback Method
cpg	491.77	J/molxK	957.04	Joback Method

dvisc	0.0013511	Paxs	422.63	Joback Method
dvisc	0.0008160	Paxs	468.54	Joback Method
dvisc	0.0005392	Paxs	514.45	Joback Method
dvisc	0.0003813	Paxs	560.36	Joback Method
dvisc	0.0002842	Paxs	606.27	Joback Method
dvisc	0.0002208	Paxs	652.18	Joback Method
dvisc	0.0001773	Paxs	698.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2001298&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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