

Alpha-p-bromo-benzohydryl-acetophenone

Inchi:	InChI=1S/C21H17BrO/c22-19-13-11-17(12-14-19)20(16-7-3-1-4-8-16)15-21(23)18-9-5-2
InchiKey:	WTKRBWMQAHGKHB-UHFFFAOYSA-N
Formula:	C21H17BrO
SMILES:	O=C(CC(c1ccccc1)c1ccc(Br)cc1)c1ccccc1
Mol. weight [g/mol]:	365.26
CAS:	5472-01-5

Physical Properties

Property code	Value	Unit	Source
gf	336.50	kJ/mol	Joback Method
hf	129.82	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.854		Crippen Method
mcvol	254.540	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	884.49	K	Joback Method
tc	1153.67	K	Joback Method
tf	512.94	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.68	J/molxK	884.49	Joback Method
cpg	722.91	J/molxK	929.35	Joback Method
cpg	735.84	J/molxK	974.22	Joback Method
cpg	747.64	J/molxK	1019.08	Joback Method
cpg	758.48	J/molxK	1063.94	Joback Method
cpg	768.54	J/molxK	1108.81	Joback Method
cpg	777.97	J/molxK	1153.67	Joback Method
dvisc	0.0007342	Paxs	512.94	Joback Method
dvisc	0.0003988	Paxs	574.87	Joback Method

dvisc	0.0002440	Paxs	636.79	Joback Method
dvisc	0.0001628	Paxs	698.72	Joback Method
dvisc	0.0001161	Paxs	760.64	Joback Method
dvisc	0.0000871	Paxs	822.57	Joback Method
dvisc	0.0000680	Paxs	884.49	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=C5472015&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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