

2-Bromoisobutyrophenone

Other names:	«alpha»-Bromoisobutyrophenone 1-Propanone, 2-bromo-2-methyl-1-phenyl- Phenyl 2-bromo-2-propyl ketone
Inchi:	InChI=1S/C10H11BrO/c1-10(2,11)9(12)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey:	QMOSZSHTSOWPRX-UHFFFAOYSA-N
Formula:	C10H11BrO
SMILES:	CC(C)(Br)C(=O)c1ccccc1
Mol. weight [g/mol]:	227.10
CAS:	10409-54-8

Physical Properties

Property code	Value	Unit	Source
gf	33.97	kJ/mol	Joback Method
hf	-108.20	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.043		Crippen Method
mcvol	147.070	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	571.68	K	Joback Method
tc	816.07	K	Joback Method
tf	341.03	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.35	J/mol×K	571.68	Joback Method
cpg	375.68	J/mol×K	775.34	Joback Method
cpg	366.18	J/mol×K	734.61	Joback Method
cpg	355.79	J/mol×K	693.88	Joback Method
cpg	344.42	J/mol×K	653.14	Joback Method
cpg	331.97	J/mol×K	612.41	Joback Method

cpg	384.38	J/mol×K	816.07	Joback Method
dvisc	0.0002496	Pa×s	571.68	Joback Method
dvisc	0.0003236	Pa×s	533.24	Joback Method
dvisc	0.0004366	Pa×s	494.80	Joback Method
dvisc	0.0006197	Pa×s	456.36	Joback Method
dvisc	0.0009381	Pa×s	417.91	Joback Method
dvisc	0.0015446	Pa×s	379.47	Joback Method
dvisc	0.0028456	Pa×s	341.03	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=C10409548&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

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