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

Physical Properties

Property code	Value	Unit	Source
af	0.4408		Cheméo Relay (1.0)
gf	33.97	kJ/mol	Joback Method
hf	-103.14	kJ/mol	Cheméo Relay (1.0)
hfus	15.17	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	3.043		Crippen Method
mcvol	147.070	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	524.71	K	Cheméo Relay (1.0)
tc	750.55	K	Cheméo Relay (1.0)
tf	314.29	K	Cheméo Relay (1.0)
vc	0.522	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	375.68	J/mol×K	775.34	Joback Method
cpg	384.38	J/mol×K	816.07	Joback Method
dvisc	0.0028456	Pa×s	341.03	Joback Method
dvisc	0.0015446	Pa×s	379.47	Joback Method
dvisc	0.0009381	Pa×s	417.91	Joback Method
dvisc	0.0006197	Pa×s	456.36	Joback Method
dvisc	0.0004366	Pa×s	494.80	Joback Method
dvisc	0.0003236	Pa×s	533.24	Joback Method
dvisc	0.0002496	Pa×s	571.68	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10409548&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
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