

2-Bromo-2'-methoxyacetophenone

Other names:	o-Methoxy phenacylbromide 2-Methoxyphenacyl bromide Ethanone, 2-bromo-1-(2-methoxyphenyl)- «alpha»-Bromo-o-methoxyacetophenone bromomethyl 2-methoxyphenyl ketone
Inchi:	InChI=1S/C9H9BrO2/c1-12-9-5-3-2-4-7(9)8(11)6-10/h2-5H,6H2,1H3
InchiKey:	GKNCPTLOPRDYMH-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	COc1ccccc1C(=O)CBr
Mol. weight [g/mol]:	229.07
CAS:	31949-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-222.50	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.273		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	579.43	K	Joback Method
tc	811.07	K	Joback Method
tf	362.09	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/mol×K	579.43	Joback Method
cpg	302.44	J/mol×K	618.04	Joback Method
cpg	313.06	J/mol×K	656.64	Joback Method
cpg	322.96	J/mol×K	695.25	Joback Method

cpg	332.17	J/mol×K	733.85	Joback Method
cpg	340.71	J/mol×K	772.46	Joback Method
cpg	348.60	J/mol×K	811.07	Joback Method
dvisc	0.0015157	Pa×s	362.09	Joback Method
dvisc	0.0009661	Pa×s	398.31	Joback Method
dvisc	0.0006638	Pa×s	434.54	Joback Method
dvisc	0.0004832	Pa×s	470.76	Joback Method
dvisc	0.0003681	Pa×s	506.98	Joback Method
dvisc	0.0002908	Pa×s	543.21	Joback Method
dvisc	0.0002365	Pa×s	579.43	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=C31949210&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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