

2-Bromo-1-indanone

Inchi:	InChI=1S/C9H7BrO/c10-8-5-6-3-1-2-4-7(6)9(8)11/h1-4,8H,5H2
InchiKey:	UXVCSPSWUNMPMT-UHFFFAOYSA-N
Formula:	C9H7BrO
SMILES:	O=C1c2ccccc2CC1Br
Mol. weight [g/mol]:	211.06
CAS:	1775-27-5

Physical Properties

Property code	Value	Unit	Source
gf	80.16	kJ/mol	Joback Method
hf	-42.60	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.189		Crippen Method
mcvol	122.120	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
tb	577.70	K	Joback Method
tc	838.20	K	Joback Method
tf	376.09	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.83	J/molxK	577.70	Joback Method
cpg	273.63	J/molxK	621.12	Joback Method
cpg	285.45	J/molxK	664.53	Joback Method
cpg	296.34	J/molxK	707.95	Joback Method
cpg	306.37	J/molxK	751.37	Joback Method
cpg	315.60	J/molxK	794.78	Joback Method
cpg	324.07	J/molxK	838.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1775275&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
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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