1H-Inden-1-one, 5-bromo-2,3-dihydro-

Other names: 1-Indanone, 5-bromo-
5-Bromo-1-indanone
5-Bromoindanone
Inchi: InChI=1S/C9H7BrO/c10-7-2-3-8-6(5-7)1-4-9(8)11/h2-3,5H,1,4H2
InchiKey: KSONICAHAPRCMV-UHFFFAOYSA-N
Formula: C9H7BrO
SMILES: O=C1CCc2cc(Br)ccc21
Mol. weight [g/mol]: 211.06
CAS: 34598-49-7

Physical Properties

Property code	Value	Unit	Source
gf	78.24	kJ/mol	Joback Method
hf	-33.73	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.578		Crippen Method
mcvol	122.120	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	587.35	K	Joback Method
tc	848.79	K	Joback Method
tf	392.85	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.42	J/mol×K	587.35	Joback Method
cpg	269.38	J/mol×K	630.92	Joback Method
cpg	280.43	J/mol×K	674.50	Joback Method
cpg	290.64	J/mol×K	718.07	Joback Method
cpg	300.06	J/mol×K	761.64	Joback Method
cpg	308.76	J/mol×K	805.22	Joback Method

cpg	316.79	J/mol×K	848.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34598497&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