5-Bromo-1-indanone

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

Physical Properties

Property code	Value	Unit	Source
hfus	14.19	kJ/mol	Joback Method
ie	9.13	eV	Cheméo Relay (1.0)
logp	2.578		Crippen Method
mcvol	122.120	ml/mol	McGowan Method
tb	564.76	K	Cheméo Relay (1.0)
tf	358.32	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34598497&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point