

4-Bromo-7-methoxy-1-oxo-indene

Inchi:	InChI=1S/C10H7BrO2/c1-13-9-5-3-7(11)6-2-4-8(12)10(6)9/h2-5H,1H3
InchiKey:	BCINXSXOEXUWKU-UHFFFAOYSA-N
Formula:	C10H7BrO2
SMILES:	<chem>COc1ccc(Br)c2c1C(=O)C=C2</chem>
Mol. weight [g/mol]:	239.06
CAS:	116373-87-6

Physical Properties

Property code	Value	Unit	Source
gf	1.99	kJ/mol	Joback Method
hf	-140.28	kJ/mol	Joback Method
hfus	18.80	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.667		Crippen Method
mcvol	137.780	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	636.79	K	Joback Method
tc	891.28	K	Joback Method
tf	439.63	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.18	J/molxK	636.79	Joback Method
cpg	314.39	J/molxK	679.20	Joback Method
cpg	324.83	J/molxK	721.62	Joback Method
cpg	334.53	J/molxK	764.03	Joback Method
cpg	343.51	J/molxK	806.45	Joback Method
cpg	351.79	J/molxK	848.86	Joback Method
cpg	359.41	J/molxK	891.28	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C116373876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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