4-Bromophenyl cyclopropyl ketone

Other names: (4-Bromophenyl)cyclopropylmethanone
Methanone, (4-bromophenyl)cyclopropyl-
Inchi: InChI=1S/C10H9BrO/c11-9-5-3-8(4-6-9)10(12)7-1-2-7/h3-7H,1-2H2
InchiKey: QTHHOINSCNBYQO-UHFFFAOYSA-N
Formula: C10H9BrO
SMILES: O=C(c1ccc(Br)cc1)C1CC1
Mol. weight [g/mol]: 225.08
CAS: 6952-89-2

Physical Properties

Property code	Value	Unit	Source
gf	82.25	kJ/mol	Joback Method
hf	-38.12	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	53.89	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.042		Crippen Method
mcvol	136.210	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	1653.00		NIST Webbook
tb	586.63	K	Joback Method
tc	834.67	K	Joback Method
tf	369.07	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.73	J/mol×K	586.63	Joback Method
cpg	311.73	J/mol×K	627.97	Joback Method
cpg	323.64	J/mol×K	669.31	Joback Method
cpg	334.55	J/mol×K	710.65	Joback Method
cpg	344.57	J/mol×K	751.99	Joback Method
cpg	353.80	J/mol×K	793.33	Joback Method

cpg	362.34	J/mol×K	834.67	Joback Method
dvisc	0.0022041	Pa×s	369.07	Joback Method
dvisc	0.0016282	Pa×s	405.33	Joback Method
dvisc	0.0012641	Pa×s	441.59	Joback Method
dvisc	0.0010199	Pa×s	477.85	Joback Method
dvisc	0.0008482	Pa×s	514.11	Joback Method
dvisc	0.0007227	Pa×s	550.37	Joback Method
dvisc	0.0006281	Pa×s	586.63	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=C6952892&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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