

3-Bromocamphor

Other names:	Bicyclo[2.2.1]heptan-2-one, 3-bromo-1,7,7-trimethyl- 2-Bornanone, 3-bromo- D-«alpha»-bromocamphor Camphor bromide 3-Bromo-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one 3-Bromo-2-bornanone D-3-bromo camphor 3-bromobornan-2-one
Inchi:	InChI=1S/C10H15BrO/c1-9(2)6-4-5-10(9,3)8(12)7(6)11/h6-7H,4-5H2,1-3H3
InchiKey:	NJQADTYRAYFBJN-UHFFFAOYSA-N
Formula:	C10H15BrO
SMILES:	CC12CCC(C(Br)C1=O)C2(C)C
Mol. weight [g/mol]:	231.13
CAS:	76-29-9

Physical Properties

Property code	Value	Unit	Source
gf	8.05	kJ/mol	Joback Method
hf	-231.86	kJ/mol	Joback Method
hfus	10.17	kJ/mol	Joback Method
hvap	45.61	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.775		Crippen Method
mcvol	149.110	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	571.07	K	Joback Method
tc	818.98	K	Joback Method
tf	402.16	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.32	J/mol×K	571.07	Joback Method

cpg	386.44	J/mol×K	612.39	Joback Method
cpg	402.39	J/mol×K	653.71	Joback Method
cpg	417.49	J/mol×K	695.02	Joback Method
cpg	432.04	J/mol×K	736.34	Joback Method
cpg	446.36	J/mol×K	777.66	Joback Method
cpg	460.77	J/mol×K	818.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76299&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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