

Cyclopentanol,2-bromo-,acetate,cis-

Inchi:	InChI=1S/C7H11BrO2/c1-5(9)10-7-4-2-3-6(7)8/h6-7H,2-4H2,1H3/t6-,7+/m0/s1
InchiKey:	RWFKZZAXUPSAQT-NKWVEPMBSA-N
Formula:	C7H11BrO2
SMILES:	CC(=O)OC1CCCC1Br
Mol. weight [g/mol]:	207.06
CAS:	53093-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-182.70	kJ/mol	Joback Method
hf	-366.14	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
ie	10.00 ± 0.02	eV	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.865		Crippen Method
mcvol	123.570	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	512.62	K	Joback Method
tc	735.30	K	Joback Method
tf	307.27	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.46	J/mol×K	512.62	Joback Method
cpg	276.29	J/mol×K	549.73	Joback Method
cpg	289.34	J/mol×K	586.85	Joback Method
cpg	301.63	J/mol×K	623.96	Joback Method
cpg	313.18	J/mol×K	661.07	Joback Method
cpg	324.00	J/mol×K	698.19	Joback Method
cpg	334.10	J/mol×K	735.30	Joback Method
dvisc	0.0023129	Paxs	307.27	Joback Method

dvisc	0.0015206	Paxs	341.50	Joback Method
dvisc	0.0010791	Paxs	375.72	Joback Method
dvisc	0.0008109	Paxs	409.94	Joback Method
dvisc	0.0006368	Paxs	444.17	Joback Method
dvisc	0.0005177	Paxs	478.39	Joback Method
dvisc	0.0004326	Paxs	512.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C53093417&Units=SI

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
ie:	Ionization energy
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

Latest version available from:

<https://www.chemeo.com/cid/25-228-1/Cyclopentanol-2-bromo-acetate-cis.pdf>

Generated by Cheméo on 2024-05-03 11:35:27.814907904 +0000 UTC m=+17025376.735485219.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.