7,7-Dichlorobicyclo(3,2,0)hept-2-en-6-one

Other names: Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dichloro-
7,7-dichlorobicyclo[3.2.0]hept-2-en-6-one
Inchi: InChI=1S/C7H6Cl2O/c8-7(9)5-3-1-2-4(5)6(7)10/h1,3-5H,2H2
InchiKey: JBPBARAOHIDZPU-UHFFFAOYSA-N
Formula: C7H6Cl2O
SMILES: O=C1C2CC=CC2C1(Cl)Cl
Mol. weight [g/mol]: 177.03
CAS: 5307-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-12.23	kJ/mol	Joback Method
hf	-164.87	kJ/mol	Joback Method
hfus	11.95	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.935		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	514.72	K	Joback Method
tc	763.85	K	Joback Method
tf	349.49	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.72	J/mol×K	514.72	Joback Method
cpg	240.88	J/mol×K	556.24	Joback Method
cpg	251.97	J/mol×K	597.76	Joback Method
cpg	262.16	J/mol×K	639.29	Joback Method
cpg	271.64	J/mol×K	680.81	Joback Method
cpg	280.58	J/mol×K	722.33	Joback Method
cpg	289.17	J/mol×K	763.85	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=C5307993&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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