

(1,4,5,6,7,7-Hexachlorobicyclo[2.2.1]hept-5-en-2-y

Inchi: InChI=1S/C8H6Cl6O/c9-4-5(10)7(12)3(2-15)1-6(4,11)8(7,13)14/h3,15H,1-2H2
InchiKey: JFSYHGUBAXUJEV-UHFFFAOYSA-N
Formula: C8H6Cl6O
SMILES: OCC1CC2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]: 330.85

Physical Properties

Property code	Value	Unit	Source
gf	-103.71	kJ/mol	Joback Method
hf	-275.80	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.831		Crippen Method
mcvol	176.870	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	717.45	K	Joback Method
tc	959.69	K	Joback Method
tf	541.64	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.21	J/molxK	717.45	Joback Method
cpg	381.19	J/molxK	757.82	Joback Method
cpg	389.89	J/molxK	798.20	Joback Method
cpg	399.76	J/molxK	838.57	Joback Method
cpg	411.22	J/molxK	878.94	Joback Method
cpg	424.71	J/molxK	919.32	Joback Method
cpg	440.68	J/molxK	959.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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