2,3,4,4,5,6-Hexabromo-2,5-cyclohexadien-1-one

Inchi: InChI=1S/C6Br6O/c7-1-3(13)2(8)5(10)6(11,12)4(1)9
InchiKey: OOROIZJCIRNLTR-UHFFFAOYSA-N
Formula: C6Br6O
SMILES: O=C1C(Br)=C(Br)C(Br)(Br)C(Br)=C1Br
Mol. weight [g/mol]: 567.49
CAS: 34946-84-4

Physical Properties

Property code	Value	Unit	Source
gf	3.33	kJ/mol	Joback Method
hf	-7.65	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.058		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	8525.96	kPa	Joback Method
tb	839.49	K	Joback Method
tc	1167.74	K	Joback Method
tf	667.28	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.83	J/mol×K	839.49	Joback Method
cpg	282.94	J/mol×K	894.20	Joback Method
cpg	291.13	J/mol×K	948.91	Joback Method
cpg	300.76	J/mol×K	1003.62	Joback Method
cpg	312.20	J/mol×K	1058.33	Joback Method
cpg	325.80	J/mol×K	1113.03	Joback Method
cpg	341.94	J/mol×K	1167.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34946844&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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