2,4,6-Tribromo-2,5-cyclohexadienone

Other names: 2,4,4,6-tetrabromocyclohexa-2,5-dienone
Inchi: InChI=1S/C6H3Br3O/c7-3-1-4(8)6(10)5(9)2-3/h1-3H
InchiKey: FZANYOHKIPVTGC-UHFFFAOYSA-N
Formula: C6H2Br4O
SMILES: O=C1C(Br)=CC(Br)C=C1Br
Mol. weight [g/mol]: 409.69
CAS: 20244-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-14.88	kJ/mol	Joback Method
hf	-78.94	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.890		Crippen Method
mcvol	130.010	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
tb	630.81	K	Joback Method
tc	915.07	K	Joback Method
tf	438.94	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.51	J/mol×K	630.81	Joback Method
cpg	232.02	J/mol×K	678.19	Joback Method
cpg	239.83	J/mol×K	725.56	Joback Method
cpg	246.93	J/mol×K	772.94	Joback Method
cpg	253.34	J/mol×K	820.32	Joback Method
cpg	259.08	J/mol×K	867.69	Joback Method
cpg	264.15	J/mol×K	915.07	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=C20244615&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