4-Dichloromethyl-4-methyl-2,5-cyclohexadien-1-o

Other names: 4-Dichloromethyl-4-methyl-2,5-cyclohexadienone
2,5-Cyclohexadien-1-one, 4-(dichloromethyl)-4-methyl-
6-Dichloromethyl-6-methyl-1,4--cyclohexadien-3-one
Inchi: InChI=1S/C8H8Cl2O/c1-8(7(9)10)4-2-6(11)3-5-8/h2-5,7H,1H3
InchiKey: MJRRCEHODULPAV-UHFFFAOYSA-N
Formula: C8H8Cl2O
SMILES: CC1(C(Cl)Cl)C=CC(=O)C=C1
Mol. weight [g/mol]: 191.06
CAS: 6611-78-5

Physical Properties

Property code	Value	Unit	Source
chs	-4130.20	kJ/mol	NIST Webbook
gf	-53.53	kJ/mol	Joback Method
hf	-197.79	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.491		Crippen Method
mcvol	130.170	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	542.79	K	Joback Method
tc	794.55	K	Joback Method
tf	325.78	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.99	J/mol×K	542.79	Joback Method
cpg	279.83	J/mol×K	584.75	Joback Method
cpg	291.73	J/mol×K	626.71	Joback Method
cpg	302.83	J/mol×K	668.67	Joback Method
cpg	313.27	J/mol×K	710.63	Joback Method

cpg	323.18	J/mol×K	752.59	Joback Method
cpg	332.70	J/mol×K	794.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6611785&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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