6-Chloro-4-chromanone

Other names:	4H-1-Benzopyran-4-one, 6-chloro-2,3-dihydro- 6-chlorochroman-4-one
Inchi:	InChI=1S/C9H7ClO2/c10-6-1-2-9-7(5-6)8(11)3-4-12-9/h1-2,5H,3-4H2
InchiKey:	LLTDYHFVIVSQPJ-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	O=C1CCOc2ccc(Cl)cc21
Mol. weight [g/mol]:	160.26
CAS:	37674-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.23	kJ/mol	Joback Method
hf	-213.96	kJ/mol	Joback Method
hfus	18.98	kJ/mol	Joback Method
hvap	52.76	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.305		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	589.84	K	Joback Method
tc	846.40	K	Joback Method
tf	236.30 ± 1.00	K	NIST Webbook
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.73	J/mol×K	589.84	Joback Method
cpg	287.30	J/mol×K	632.60	Joback Method
cpg	298.97	J/mol×K	675.36	Joback Method
cpg	309.76	J/mol×K	718.12	Joback Method
cpg	319.70	J/mol×K	760.88	Joback Method
cpg	328.82	J/mol×K	803.64	Joback Method
cpg	337.13	J/mol×K	846.40	Joback Method

Sources

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=C37674729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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