3-Cl-4-CH3O-C6H3-CCH

Inchi: InChI=1S/C9H7ClO/c1-3-7-4-5-9(11-2)8(10)6-7/h1,4-6H,2H3
InchiKey: CQJNAMMLEBMXFO-UHFFFAOYSA-N
Formula: C9H7ClO
SMILES: C#Cc1ccc(OC)c(Cl)c1
Mol. weight [g/mol]: 166.60
CAS: 120136-29-0

Physical Properties

Property code	Value	Unit	Source
affp	871.90	kJ/mol	NIST Webbook
basg	839.50	kJ/mol	NIST Webbook
gf	224.19	kJ/mol	Joback Method
hf	128.44	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	45.88	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.330		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	491.93	K	Joback Method
tc	722.66	K	Joback Method
tf	341.77	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.10	J/mol×K	491.93	Joback Method
cpg	243.53	J/mol×K	530.39	Joback Method
cpg	253.37	J/mol×K	568.84	Joback Method
cpg	262.63	J/mol×K	607.30	Joback Method
cpg	271.34	J/mol×K	645.75	Joback Method
cpg	279.52	J/mol×K	684.21	Joback Method
cpg	287.16	J/mol×K	722.66	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=C120136290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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