

Ethanone, 1-(3-chloro-4-methoxyphenyl)-

Other names:	3-Chloro-4-methoxyacetophenone 3-Cl-4-CH3O-C6H3-COCH3
Inchi:	InChI=1S/C9H9ClO2/c1-6(11)7-3-4-9(12-2)8(10)5-7/h3-5H,1-2H3
InchiKey:	QILWOKAXHOAFOF-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	COc1ccc(C(C)=O)cc1Cl
Mol. weight [g/mol]:	184.62
CAS:	37612-52-5

Physical Properties

Property code	Value	Unit	Source
affp	883.70	kJ/mol	NIST Webbook
basg	851.90	kJ/mol	NIST Webbook
gf	-127.80	kJ/mol	Joback Method
hf	-276.04	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.551		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	555.68	K	Joback Method
tc	778.87	K	Joback Method
tf	344.73	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.08	J/molxK	555.68	Joback Method
cpg	291.31	J/molxK	592.88	Joback Method
cpg	301.92	J/molxK	630.08	Joback Method
cpg	311.91	J/molxK	667.27	Joback Method
cpg	321.30	J/molxK	704.47	Joback Method

cpg	330.08	J/molxK	741.67	Joback Method
cpg	338.26	J/molxK	778.87	Joback Method
dvisc	0.0013360	Paxs	344.73	Joback Method
dvisc	0.0008629	Paxs	379.89	Joback Method
dvisc	0.0006002	Paxs	415.05	Joback Method
dvisc	0.0004418	Paxs	450.20	Joback Method
dvisc	0.0003399	Paxs	485.36	Joback Method
dvisc	0.0002710	Paxs	520.52	Joback Method
dvisc	0.0002223	Paxs	555.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37612525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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