

Cyclopropyl 4-methoxyphenyl ketone

Other names:	Methanone, cyclopropyl(4-methoxyphenyl)- Cyclopropyl(4-methoxyphenyl)methanone Cyclopropyl p-anisyl ketone
Inchi:	InChI=1S/C11H12O2/c1-13-10-6-4-9(5-7-10)11(12)8-2-3-8/h4-8H,2-3H2,1H3
InchiKey:	YKZSVEVTRUSPOQ-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	<chem>COc1ccc(C(=O)C2CC2)cc1</chem>
Mol. weight [g/mol]:	176.21
CAS:	7152-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-28.65	kJ/mol	Joback Method
hf	-217.31	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	52.09	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.288		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	565.77	K	Joback Method
tc	791.94	K	Joback Method
tf	342.77	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.55	J/molxK	565.77	Joback Method
cpg	396.47	J/molxK	754.25	Joback Method
cpg	385.26	J/molxK	716.55	Joback Method
cpg	373.21	J/molxK	678.86	Joback Method
cpg	360.28	J/molxK	641.16	Joback Method
cpg	346.41	J/molxK	603.47	Joback Method

cpg	406.89	J/mol×K	791.94	Joback Method
dvisc	0.0004407	Paxs	565.77	Joback Method
dvisc	0.0005103	Paxs	528.60	Joback Method
dvisc	0.0006042	Paxs	491.44	Joback Method
dvisc	0.0007355	Paxs	454.27	Joback Method
dvisc	0.0009272	Paxs	417.10	Joback Method
dvisc	0.0012230	Paxs	379.94	Joback Method
dvisc	0.0017132	Paxs	342.77	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=C7152036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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