Cyclopropyl-4-methoxyphenylketone

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: COc1ccc(C(=O)C2CC2)cc1
Mol. weight [g/mol]: 176.22

Physical Properties

Property code	Value	Unit	Source
hf	-180.25	kJ/mol	Cheméo Relay (1.0)
hfus	18.82	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	2.288		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
tb	561.40	K	Cheméo Relay (1.0)
tf	340.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.55	J/mol×K	565.77	Joback Method
cpg	346.41	J/mol×K	603.47	Joback Method
cpg	360.28	J/mol×K	641.16	Joback Method
cpg	373.21	J/mol×K	678.86	Joback Method
cpg	385.26	J/mol×K	716.55	Joback Method
cpg	396.47	J/mol×K	754.25	Joback Method
cpg	406.89	J/mol×K	791.94	Joback Method
dvisc	0.0017132	Pa×s	342.77	Joback Method
dvisc	0.0012230	Pa×s	379.94	Joback Method
dvisc	0.0009272	Pa×s	417.10	Joback Method

dvisc	0.0007355	Pa×s	454.27	Joback Method
dvisc	0.0006042	Pa×s	491.44	Joback Method
dvisc	0.0005103	Pa×s	528.60	Joback Method
dvisc	0.0004407	Pa×s	565.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7152036&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point