

3-CH₃OC₆H₄C(CH₃)=CH₂

Inchi:	InChI=1S/C10H12O/c1-8(2)9-5-4-6-10(7-9)11-3/h4-7H,1H2,2-3H3
InchiKey:	WTPHVMQZKICGOH-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	C=C(C)c1cccc(OC)c1
Mol. weight [g/mol]:	148.20
CAS:	25108-57-0

Physical Properties

Property code	Value	Unit	Source
affp	872.60	kJ/mol	NIST Webbook
basg	843.70	kJ/mol	NIST Webbook
gf	110.39	kJ/mol	Joback Method
hf	-41.25	kJ/mol	Joback Method
hfus	13.91	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.728		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	478.84	K	Joback Method
tc	691.84	K	Joback Method
tf	247.91	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.20	J/mol×K	478.84	Joback Method
cpg	278.05	J/mol×K	514.34	Joback Method
cpg	291.18	J/mol×K	549.84	Joback Method
cpg	303.60	J/mol×K	585.34	Joback Method
cpg	315.35	J/mol×K	620.84	Joback Method
cpg	326.43	J/mol×K	656.34	Joback Method
cpg	336.87	J/mol×K	691.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25108570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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