

Ethanone, 1-[4-(1-methyl-2-propenyl)phenyl]-

Other names:	1-[4-(1-Methyl-2-propenyl)phenyl]ethanone
Inchi:	InChI=1S/C12H14O/c1-4-9(2)11-5-7-12(8-6-11)10(3)13/h4-9H,1H2,2-3H3
InchiKey:	PGFYBSVJKSNEJQ-UHFFFAOYSA-N
Formula:	C12H14O
SMILES:	C=CC(C)c1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	174.24
CAS:	109586-49-4

Physical Properties

Property code	Value	Unit	Source
gf	109.42	kJ/mol	Joback Method
hf	-58.38	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.179		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1883.00		NIST Webbook
tb	555.73	K	Joback Method
tc	773.97	K	Joback Method
tf	297.11	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.98	J/mol×K	555.73	Joback Method
cpg	363.98	J/mol×K	592.10	Joback Method
cpg	378.05	J/mol×K	628.48	Joback Method
cpg	391.24	J/mol×K	664.85	Joback Method
cpg	403.57	J/mol×K	701.23	Joback Method
cpg	415.09	J/mol×K	737.60	Joback Method
cpg	425.84	J/mol×K	773.97	Joback Method

dvisc	0.0027861	Pa×s	297.11	Joback Method
dvisc	0.0013837	Pa×s	340.21	Joback Method
dvisc	0.0008043	Pa×s	383.32	Joback Method
dvisc	0.0005217	Pa×s	426.42	Joback Method
dvisc	0.0003664	Pa×s	469.52	Joback Method
dvisc	0.0002731	Pa×s	512.63	Joback Method
dvisc	0.0002130	Pa×s	555.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C109586494&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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