3,4-Methylenedioxybenzylidene acetone

Other names:	Piperonylideneacetone
	1-(3,4-Methylenedioxyphenyl)but-2-en-3-one
	3-Buten-2-one, 4-(1,3-benzodioxol-5-yl)-
	Acetone, piperonylidene-
	Heliotropyl acetone
	Piperonyl acetone
	Piperonalacetone
	3-Buten-2-one, 4-(3,4-(methylenedioxy)phenyl)-
	NSC 217304
	NSC 407384
	2-Butanone, 4-(3,4-(methylenedioxy)phenyl)-
	4-(3,4-methylenedioxyphenyl)but-3-en-2-one
Inchi:	InChI=1S/C11H10O3/c1-8(12)2-3-9-4-5-10-11(6-9)14-7-13-10/h2-6H,7H2,1H3/b3-2+
InchiKey:	XIYPXOFSURQTTJ-NSCUHMNNSA-N
Formula:	C11H10O3
SMILES:	CC(=O)C=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	190.20
CAS:	3160-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.59	kJ/mol	Joback Method
hf	-223.00	kJ/mol	Joback Method
hfus	32.33	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.017		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	611.06	K	Joback Method
tc	846.05	K	Joback Method
tf	385.36	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.70	J/mol×K	611.06	Joback Method
cpg	394.93	J/mol×K	806.89	Joback Method
cpg	385.83	J/mol×K	767.72	Joback Method
cpg	376.04	J/mol×K	728.56	Joback Method
cpg	365.48	J/mol×K	689.39	Joback Method
cpg	354.06	J/mol×K	650.23	Joback Method
cpg	403.44	J/mol×K	846.05	Joback Method
dvisc	0.0004003	Pa×s	611.06	Joback Method
dvisc	0.0004797	Pa×s	573.44	Joback Method
dvisc	0.0005896	Pa×s	535.83	Joback Method
dvisc	0.0007476	Pa×s	498.21	Joback Method
dvisc	0.0009855	Pa×s	460.59	Joback Method
dvisc	0.0013645	Pa×s	422.98	Joback Method
dvisc	0.0020131	Pa×s	385.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3160370&Units=SI
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

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