

2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2,5-dimethyl-

Other names:	Methacrolein dimer Methacrylaldehyde dimer 1,4-Pyran, 2,3-dihydro-2,5-dimethyl-2-formyl- 2,3-Dihydro-2,5-dimethyl-2-formyl-1,4-pyran 2,3-Dihydro-2,5-dimethyl-2H-pyran-2-carboxaldehyde 2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2,5-dimethylmethacrolein dimer 3,4-dihydro-2,5-dimethyl-2H-pyran-2-carbaldehyde
Inchi:	InChI=1S/C8H12O2/c1-7-3-4-8(2,6-9)10-5-7/h5-6H,3-4H2,1-2H3
InchiKey:	DYVJZCIYRQUXBA-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC1=COC(C)(C=O)CC1
Mol. weight [g/mol]:	140.18
CAS:	1920-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-129.87	kJ/mol	Joback Method
hf	-310.16	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	481.98	K	Joback Method
tc	701.29	K	Joback Method
tf	209.00 ± 0.60	K	NIST Webbook
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.70	J/mol×K	481.98	Joback Method
cpg	268.57	J/mol×K	518.53	Joback Method

cpg	281.47	J/mol×K	555.08	Joback Method
cpg	293.50	J/mol×K	591.63	Joback Method
cpg	304.77	J/mol×K	628.19	Joback Method
cpg	315.38	J/mol×K	664.74	Joback Method
cpg	325.44	J/mol×K	701.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1920214&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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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