Octanal, 7-methoxy-3,7-dimethyl-

Other names:	Methoxycitronellal
	7-Methoxy-3,7-dimethyloctanal
	3,7-Dimethyl-7-methoxy-1-octanal
	1-Octanal, 3,7-dimethyl-7-methoxy-
	Hydroxycitronellal methyl ether
Inchi:	InChI=1S/C11H22O2/c1-10(7-9-12)6-5-8-11(2,3)13-4/h9-10H,5-8H2,1-4H3
InchiKey:	IDWULKZGRNHZNR-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	COC(C)(C)CCCC(C)CC=O
Mol. weight [g/mol]:	186.29
CAS:	3613-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-162.38	kJ/mol	Joback Method
hf	-502.20	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.807		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
ripol	1839.00		NIST Webbook
ripol	1839.00		NIST Webbook
tb	518.49	K	Joback Method
tc	698.36	K	Joback Method
tf	265.38	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.67	J/mol×K	518.49	Joback Method
cpg	491.34	J/mol×K	668.38	Joback Method

cpg	478.20	J/mol×K	638.40	Joback Method
cpg	464.38	J/mol×K	608.42	Joback Method
cpg	449.87	J/mol×K	578.45	Joback Method
cpg	434.64	J/mol×K	548.47	Joback Method
cpg	503.83	J/mol×K	698.36	Joback Method
dvisc	0.0002012	Pa×s	518.49	Joback Method
dvisc	0.0002802	Pa×s	476.31	Joback Method
dvisc	0.0004161	Pa×s	434.12	Joback Method
dvisc	0.0006730	Pa×s	391.94	Joback Method
dvisc	0.0012224	Pa×s	349.75	Joback Method
dvisc	0.0026152	Pa×s	307.56	Joback Method
dvisc	0.0071253	Pa×s	265.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	0.05	NIST Webbook

Sources

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=C3613307&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume