6-Octen-1-ol, 3,7-dimethyl-, formate

Other names:	2,6-Dimethyl-2-octen-8-yl formate
	3,7-Dimethyl-6-octen-1-yl formate
	Citronellyl formate
	Citronelyl formate
	Formic acid, 3,7-dimethyl-6-octen-1-yl ester
	Formic acid, citronellyl ester
Inchi:	InChI=1S/C11H20O2/c1-10(2)5-4-6-11(3)7-8-13-9-12/h5,9,11H,4,6-8H2,1-3H3
InchiKey:	DZNVIZQPWLDQHI-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CC(C)=CCCC(C)CCOC=O
Mol. weight [g/mol]:	184.28
CAS:	105-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.55	kJ/mol	Joback Method
hf	-386.02	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.932		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1285.50		NIST Webbook
rinpol	1258.90		NIST Webbook

rinpol	1256.20	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1255.60	NIST Webbook
rinpol	1285.50	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1256.20	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1255.60	NIST Webbook
rinpol	1216.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1273.00	NIST Webbook
ripol	1629.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1629.00	NIST Webbook
ripol	1636.00	NIST Webbook
ripol	1600.00	NIST Webbook
ripol	1600.00	NIST Webbook
ripol	1605.00	NIST Webbook
ripol	1625.00	NIST Webbook
ripol	1615.00	NIST Webbook
ripol	1644.00	NIST Webbook
ripol	1599.00	NIST Webbook
ripol	1600.00	NIST Webbook
ripol	1605.00	NIST Webbook
ripol	1616.00	NIST Webbook
ripol	1612.90	NIST Webbook

ripol	1588.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1644.00		NIST Webbook
tb	525.76	K	Joback Method
tc	706.19	K	Joback Method
tf	243.92	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.92	J/mol×K	525.76	Joback Method
cpg	412.75	J/mol×K	555.83	Joback Method
cpg	426.94	J/mol×K	585.90	Joback Method
cpg	440.49	J/mol×K	615.98	Joback Method
cpg	453.43	J/mol×K	646.05	Joback Method
cpg	465.77	J/mol×K	676.12	Joback Method
cpg	477.54	J/mol×K	706.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65377e+01
Coeff. B	-4.97929e+03
Coeff. C	-8.36470e+01
Temperature range (K), min.	390.06
Temperature range (K), max.	527.19

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=C105851&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/89-395-6/6-Octen-1-ol-3-7-dimethyl-formate.pdf

Generated by Cheméo on 2024-10-12 08:34:56.288054786 +0000 UTC m=+3302958.925024033.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.