

Ethanal methyl nonyl acetal

Inchi:	InChI=1S/C12H26O2/c1-4-5-6-7-8-9-10-11-14-12(2)13-3/h12H,4-11H2,1-3H3
InchiKey:	KLZGMJZMJBGSMW-UHFFFAOYSA-N
Formula:	C12H26O2
SMILES:	CCCCCCCCCOC(C)OC
Mol. weight [g/mol]:	202.33

Physical Properties

Property code	Value	Unit	Source
gf	-162.28	kJ/mol	Joback Method
hf	-560.73	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.746		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1352.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1621.00		NIST Webbook
tb	518.36	K	Joback Method
tc	682.34	K	Joback Method
tf	254.46	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.54	J/molxK	518.36	Joback Method
cpg	481.08	J/molxK	545.69	Joback Method
cpg	497.06	J/molxK	573.02	Joback Method
cpg	512.48	J/molxK	600.35	Joback Method
cpg	527.34	J/molxK	627.68	Joback Method
cpg	541.66	J/molxK	655.01	Joback Method

cpg	555.42	J/molxK	682.34	Joback Method
dvisc	0.0042647	Paxs	254.46	Joback Method
dvisc	0.0015728	Paxs	298.44	Joback Method
dvisc	0.0007494	Paxs	342.43	Joback Method
dvisc	0.0004228	Paxs	386.41	Joback Method
dvisc	0.0002681	Paxs	430.39	Joback Method
dvisc	0.0001850	Paxs	474.38	Joback Method
dvisc	0.0001359	Paxs	518.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409795&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
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/37-346-7/Ethanal-methyl-nonyl-acetal.pdf>

Generated by Cheméo on 2024-04-20 05:23:57.661554677 +0000 UTC m=+15879886.582131988.

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