Octanal dimethyl acetal

Other names: Octane, 1,1-dimethoxy-
n-Octanal dimethyl acetal
1,1-Dimethoxyoctane
Inchi: InChI=1S/C10H22O2/c1-4-5-6-7-8-9-10(11-2)12-3/h10H,4-9H2,1-3H3
InchiKey: BZOOCKAFKVYAOZ-UHFFFAOYSA-N
Formula: C10H22O2
SMILES: CCCCCCCC(OC)OC
Mol. weight [g/mol]: 174.28
CAS: 10022-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-179.12	kJ/mol	Joback Method
hf	-519.45	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.966		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1162.80		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1162.80		NIST Webbook
ripol	1366.00		NIST Webbook
tb	472.60	K	Joback Method
tc	638.49	K	Joback Method
tf	231.92	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.40	J/mol×K	472.60	Joback Method
cpg	439.18	J/mol×K	610.84	Joback Method

cpg	426.16	J/mol×K	583.19	Joback Method
cpg	412.67	J/mol×K	555.54	Joback Method
cpg	398.71	J/mol×K	527.90	Joback Method
cpg	384.29	J/mol×K	500.25	Joback Method
cpg	451.74	J/mol×K	638.49	Joback Method
dvisc	0.0001614	Pa×s	472.60	Joback Method
dvisc	0.0002182	Pa×s	432.49	Joback Method
dvisc	0.0003135	Pa×s	392.37	Joback Method
dvisc	0.0004893	Pa×s	352.26	Joback Method
dvisc	0.0008564	Pa×s	312.15	Joback Method
dvisc	0.0017676	Pa×s	272.03	Joback Method
dvisc	0.0046878	Pa×s	231.92	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10022283&Units=SI

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