Octane, 1,1-diethoxy-

Other names: Octanal diethyl acetal
1,1-Diethoxyoctane
n-Octanal diethyl acetal
Inchi: InChI=1S/C12H26O2/c1-4-7-8-9-10-11-12(13-5-2)14-6-3/h12H,4-11H2,1-3H3
InchiKey: BRKIPAWFUDCCOO-UHFFFAOYSA-N
Formula: C12H26O2
SMILES: CCCCCCCC(OCC)OCC
Mol. weight [g/mol]: 202.33
CAS: 54889-48-4

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	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1276.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1431.00		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/mol×K	518.36	Joback Method

cpg	481.08	J/mol×K	545.69	Joback Method
cpg	497.06	J/mol×K	573.02	Joback Method
cpg	512.48	J/mol×K	600.35	Joback Method
cpg	527.34	J/mol×K	627.68	Joback Method
cpg	541.66	J/mol×K	655.01	Joback Method
cpg	555.42	J/mol×K	682.34	Joback Method
dvisc	0.0042647	Pa×s	254.46	Joback Method
dvisc	0.0015728	Pa×s	298.44	Joback Method
dvisc	0.0007494	Pa×s	342.43	Joback Method
dvisc	0.0004228	Pa×s	386.41	Joback Method
dvisc	0.0002681	Pa×s	430.39	Joback Method
dvisc	0.0001850	Pa×s	474.38	Joback Method
dvisc	0.0001359	Pa×s	518.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54889484&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