

1,1-diethoxyhexadecane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H42O2/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21-5-2)22-6-3/h20H

YURMTKBNIXEQDJ-UHFFFAOYSA-N

C20H42O2

CCCCCCCCCCCCCCCC(OCC)OCC

314.55

Physical Properties

Property code	Value	Unit	Source
gf	-94.92	kJ/mol	Joback Method
hf	-725.85	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.867		Crippen Method
mcvol	304.400	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
ripol	2231.00		NIST Webbook
ripol	2231.00		NIST Webbook
tb	701.40	K	Joback Method
tc	866.89	K	Joback Method
tf	344.62	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.24	J/mol×K	701.40	Joback Method
cpg	930.01	J/mol×K	728.98	Joback Method
cpg	949.89	J/mol×K	756.56	Joback Method
cpg	968.88	J/mol×K	784.15	Joback Method
cpg	987.01	J/mol×K	811.73	Joback Method
cpg	1004.28	J/mol×K	839.31	Joback Method
cpg	1020.71	J/mol×K	866.89	Joback Method
dvisc	0.0020434	Pa×s	344.62	Joback Method

dvisc	0.0007100	Pa×s	404.08	Joback Method
dvisc	0.0003235	Pa×s	463.55	Joback Method
dvisc	0.0001763	Pa×s	523.01	Joback Method
dvisc	0.0001087	Pa×s	582.47	Joback Method
dvisc	0.0000733	Pa×s	641.94	Joback Method
dvisc	0.0000529	Pa×s	701.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340691&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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