

1,1-diethoxyheptadecane

Inchi:	InChI=1S/C21H44O2/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22-5-2)23-6-3/h2
InchiKey:	QJKRDGVHGFSQL-UHFFFAOYSA-N
Formula:	C21H44O2
SMILES:	CCCCCCCCCCCCCCCC(OCC)OCC
Mol. weight [g/mol]:	328.57

Physical Properties

Property code	Value	Unit	Source
gf	-86.50	kJ/mol	Joback Method
hf	-746.49	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.257		Crippen Method
mvol	318.490	ml/mol	McGowan Method
pc	940.95	kPa	Joback Method
ripol	2347.00		NIST Webbook
ripol	2347.00		NIST Webbook
tb	724.28	K	Joback Method
tc	891.91	K	Joback Method
tf	355.89	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.42	J/molxK	724.28	Joback Method
cpg	1067.25	J/molxK	863.97	Joback Method
cpg	1049.72	J/molxK	836.03	Joback Method
cpg	1031.29	J/molxK	808.09	Joback Method
cpg	1011.94	J/molxK	780.16	Joback Method
cpg	991.65	J/molxK	752.22	Joback Method
cpg	1083.89	J/molxK	891.91	Joback Method
dvisc	0.0000461	Paxs	724.28	Joback Method

dvisc	0.0000641	Paxs	662.88	Joback Method
dvisc	0.0000952	Paxs	601.48	Joback Method
dvisc	0.0001547	Paxs	540.09	Joback Method
dvisc	0.0002848	Paxs	478.69	Joback Method
dvisc	0.0006274	Paxs	417.29	Joback Method
dvisc	0.0018154	Paxs	355.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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