

Hexadecyl pentyl ether

Inchi:	InChI=1S/C21H44O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-21-22-20-18-6-4-2/h3-21H
InchiKey:	LVEVHZZBALTDLY-UHFFFAOYSA-N
Formula:	C21H44O
SMILES:	CCCCCCCCCCCCCCCCOCCCCC
Mol. weight [g/mol]:	312.57

Physical Properties

Property code	Value	Unit	Source
gf	20.94	kJ/mol	Joback Method
hf	-608.99	kJ/mol	Joback Method
hfus	51.33	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.675		Crippen Method
mvol	312.620	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
rinpol	2172.00		NIST Webbook
tb	702.30	K	Joback Method
tc	866.33	K	Joback Method
tf	348.66	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.43	J/molxK	702.30	Joback Method
cpg	956.63	J/molxK	729.64	Joback Method
cpg	976.93	J/molxK	756.98	Joback Method
cpg	996.35	J/molxK	784.32	Joback Method
cpg	1014.91	J/molxK	811.65	Joback Method
cpg	1032.64	J/molxK	838.99	Joback Method
cpg	1049.54	J/molxK	866.33	Joback Method
dvisc	0.0021329	Paxs	348.66	Joback Method
dvisc	0.0007851	Paxs	407.60	Joback Method

dvisc	0.0003720	Paxs	466.54	Joback Method
dvisc	0.0002084	Paxs	525.48	Joback Method
dvisc	0.0001312	Paxs	584.42	Joback Method
dvisc	0.0000899	Paxs	643.36	Joback Method
dvisc	0.0000657	Paxs	702.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406418&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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