

Heptyl hexadecyl ether

Inchi:	InChI=1S/C23H48O/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-21-23-24-22-20-18-8-6-4-2/
InchiKey:	HMGCKWQTUDCOLH-UHFFFAOYSA-N
Formula:	C23H48O
SMILES:	CCCCCCCCCCCCCCCCOCCCCCCC
Mol. weight [g/mol]:	340.63

Physical Properties

Property code	Value	Unit	Source
gf	37.78	kJ/mol	Joback Method
hf	-650.27	kJ/mol	Joback Method
hfus	56.51	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	8.455		Crippen Method
mvol	340.800	ml/mol	McGowan Method
pc	843.58	kPa	Joback Method
rinpol	2365.00		NIST Webbook
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tb	748.06	K	Joback Method
tc	917.69	K	Joback Method
tf	371.20	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.80	J/molxK	748.06	Joback Method
cpg	1082.02	J/molxK	776.33	Joback Method
cpg	1103.22	J/molxK	804.60	Joback Method
cpg	1123.45	J/molxK	832.87	Joback Method
cpg	1142.71	J/molxK	861.14	Joback Method
cpg	1161.05	J/molxK	889.42	Joback Method
cpg	1178.49	J/molxK	917.69	Joback Method
dvisc	0.0017041	Paxs	371.20	Joback Method

dvisc	0.0006188	Paxs	434.01	Joback Method
dvisc	0.0002903	Paxs	496.82	Joback Method
dvisc	0.0001614	Paxs	559.63	Joback Method
dvisc	0.0001010	Paxs	622.44	Joback Method
dvisc	0.0000689	Paxs	685.25	Joback Method
dvisc	0.0000501	Paxs	748.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406394&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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