Dodecyl nonyl ether

Inchi: InChI=1S/C21H44O/c1-3-5-7-9-11-12-13-15-17-19-21-22-20-18-16-14-10-8-6-4-2/h3-21H
InchiKey: KHLXREQPFFCLSS-UHFFFAOYSA-N
Formula: C21H44O
SMILES: CCCCCCCCCCCCCOCCCCCCCCC
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
mcvol	312.620	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
tb	702.30	K	Joback Method
tc	866.33	K	Joback Method
tf	348.66	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.43	J/mol×K	702.30	Joback Method
cpg	956.63	J/mol×K	729.64	Joback Method
cpg	976.93	J/mol×K	756.98	Joback Method
cpg	996.35	J/mol×K	784.32	Joback Method
cpg	1014.91	J/mol×K	811.65	Joback Method
cpg	1032.64	J/mol×K	838.99	Joback Method
cpg	1049.54	J/mol×K	866.33	Joback Method
dvisc	0.0021329	Pa×s	348.66	Joback Method
dvisc	0.0007851	Pa×s	407.60	Joback Method
dvisc	0.0003720	Pa×s	466.54	Joback Method

dvisc	0.0002084	Pa×s	525.48	Joback Method
dvisc	0.0001312	Pa×s	584.42	Joback Method
dvisc	0.0000899	Pa×s	643.36	Joback Method
dvisc	0.0000657	Pa×s	702.30	Joback Method

Sources

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=U406375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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