Docosyl nonyl ether

Inchi: InChI=1S/C31H64O/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27-29-31-3
InchiKey: PBKCTXOYDQCDTQ-UHFFFAOYSA-N
Formula: C31H64O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOCCCCCCCCC
Mol. weight [g/mol]: 452.84

Physical Properties

Property code	Value	Unit	Source
gf	105.14	kJ/mol	Joback Method
hf	-815.39	kJ/mol	Joback Method
hfus	77.23	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-11.89		Crippen Method
logp	11.575		Crippen Method
mcvol	453.520	ml/mol	McGowan Method
pc	563.94	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	931.10	K	Joback Method
tc	1157.26	K	Joback Method
tf	461.36	K	Joback Method
vc	1.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1586.38	J/mol×K	931.10	Joback Method
cpg	1614.95	J/mol×K	968.79	Joback Method
cpg	1641.60	J/mol×K	1006.49	Joback Method
cpg	1666.45	J/mol×K	1044.18	Joback Method
cpg	1689.59	J/mol×K	1081.87	Joback Method
cpg	1711.11	J/mol×K	1119.57	Joback Method
cpg	1731.12	J/mol×K	1157.26	Joback Method
dvisc	0.0006009	Pa×s	461.36	Joback Method

dvisc	0.0002095	Pa×s	539.65	Joback Method
dvisc	0.0000954	Pa×s	617.94	Joback Method
dvisc	0.0000518	Pa×s	696.23	Joback Method
dvisc	0.0000319	Pa×s	774.52	Joback Method
dvisc	0.0000214	Pa×s	852.81	Joback Method
dvisc	0.0000154	Pa×s	931.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406379&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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