

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: CCCCCCCCCCCCCCCCCCCCCOCCCCCCCCC
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
mvol	453.520	ml/mol	McGowan Method
pc	563.94	kPa	Joback Method
rinpol	3153.00		NIST Webbook
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tb	931.10	K	Joback Method
tc	1157.26	K	Joback Method
tf	461.36	K	Joback Method
vc	1.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1586.38	J/molxK	931.10	Joback Method
cpg	1711.11	J/molxK	1119.57	Joback Method
cpg	1689.59	J/molxK	1081.87	Joback Method
cpg	1666.45	J/molxK	1044.18	Joback Method
cpg	1641.60	J/molxK	1006.49	Joback Method
cpg	1614.95	J/molxK	968.79	Joback Method
cpg	1731.12	J/molxK	1157.26	Joback Method
dvisc	0.0000154	Paxs	931.10	Joback Method

dvisc	0.0000214	Paxs	852.81	Joback Method
dvisc	0.0000319	Paxs	774.52	Joback Method
dvisc	0.0000518	Paxs	696.23	Joback Method
dvisc	0.0000954	Paxs	617.94	Joback Method
dvisc	0.0002095	Paxs	539.65	Joback Method
dvisc	0.0006009	Paxs	461.36	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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