Isopropyl octacosyl ether

Inchi: InChI=1S/C31H64O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: DPBYOVJEQQZUGS-UHFFFAOYSA-N
Formula: C31H64O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]: 452.84

Physical Properties

Property code	Value	Unit	Source
gf	102.70	kJ/mol	Joback Method
hf	-820.67	kJ/mol	Joback Method
hfus	73.71	kJ/mol	Joback Method
hvap	86.62	kJ/mol	Joback Method
log10ws	-12.00		Crippen Method
logp	11.574		Crippen Method
mcvol	453.520	ml/mol	McGowan Method
pc	566.08	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	930.66	K	Joback Method
tc	1154.47	K	Joback Method
tf	446.36	K	Joback Method
vc	1.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1586.69	J/mol×K	930.66	Joback Method
cpg	1614.93	J/mol×K	967.96	Joback Method
cpg	1641.30	J/mol×K	1005.26	Joback Method
cpg	1665.87	J/mol×K	1042.57	Joback Method
cpg	1688.75	J/mol×K	1079.87	Joback Method
cpg	1710.03	J/mol×K	1117.17	Joback Method
cpg	1729.80	J/mol×K	1154.47	Joback Method
dvisc	0.0007302	Pa×s	446.36	Joback Method

dvisc	0.0002283	Pa×s	527.08	Joback Method
dvisc	0.0000972	Pa×s	607.79	Joback Method
dvisc	0.0000505	Pa×s	688.51	Joback Method
dvisc	0.0000302	Pa×s	769.23	Joback Method
dvisc	0.0000198	Pa×s	849.94	Joback Method
dvisc	0.0000140	Pa×s	930.66	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=U406347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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