1-Docosanol, methyl ether

Inchi: InChI=1S/C23H48O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2/
InchiKey: QYXQOJNAQHQRSY-UHFFFAOYSA-N
Formula: C23H48O
SMILES: CCCCCCCCCCCCCCCCCCCCCCOC
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
mcvol	340.800	ml/mol	McGowan Method
pc	843.58	kPa	Joback Method
rinpol	2427.50		NIST Webbook
tb	748.06	K	Joback Method
tc	917.69	K	Joback Method
tf	371.20	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.80	J/mol×K	748.06	Joback Method
cpg	1082.02	J/mol×K	776.33	Joback Method
cpg	1103.22	J/mol×K	804.60	Joback Method
cpg	1123.45	J/mol×K	832.87	Joback Method
cpg	1142.71	J/mol×K	861.14	Joback Method
cpg	1161.05	J/mol×K	889.42	Joback Method
cpg	1178.49	J/mol×K	917.69	Joback Method
dvisc	0.0017041	Pa×s	371.20	Joback Method
dvisc	0.0006188	Pa×s	434.01	Joback Method

dvisc	0.0002903	Pa×s	496.82	Joback Method
dvisc	0.0001614	Pa×s	559.63	Joback Method
dvisc	0.0001010	Pa×s	622.44	Joback Method
dvisc	0.0000689	Pa×s	685.25	Joback Method
dvisc	0.0000501	Pa×s	748.06	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=U333919&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume