1-Methoxy-2,14-dimethylheptacosane

Inchi: InChI=1S/C30H62O/c1-5-6-7-8-9-10-11-13-16-19-22-25-29(2)26-23-20-17-14-12-15-18-2
InchiKey: VRRUMZGRQUTELI-UHFFFAOYSA-N
Formula: C30H62O
SMILES: CCCCCCCCCCCCCC(C)CCCCCCCCCCCC(C)COC
Mol. weight [g/mol]: 438.81

Physical Properties

Property code	Value	Unit	Source
gf	91.84	kJ/mol	Joback Method
hf	-805.31	kJ/mol	Joback Method
hfus	67.60	kJ/mol	Joback Method
hvap	84.01	kJ/mol	Joback Method
log10ws	-10.98		Crippen Method
logp	10.897		Crippen Method
mcvol	439.430	ml/mol	McGowan Method
pc	595.17	kPa	Joback Method
rinpol	3005.00		NIST Webbook
tb	907.34	K	Joback Method
tc	1118.98	K	Joback Method
tf	420.09	K	Joback Method
vc	1.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1519.32	J/mol×K	907.34	Joback Method
cpg	1546.31	J/mol×K	942.61	Joback Method
cpg	1571.61	J/mol×K	977.89	Joback Method
cpg	1595.28	J/mol×K	1013.16	Joback Method
cpg	1617.40	J/mol×K	1048.43	Joback Method
cpg	1638.05	J/mol×K	1083.71	Joback Method
cpg	1657.31	J/mol×K	1118.98	Joback Method
dvisc	0.0010616	Pa×s	420.09	Joback Method
dvisc	0.0002936	Pa×s	501.30	Joback Method

dvisc	0.0001162	Pa×s	582.51	Joback Method
dvisc	0.0000577	Pa×s	663.72	Joback Method
dvisc	0.0000334	Pa×s	744.92	Joback Method
dvisc	0.0000215	Pa×s	826.13	Joback Method
dvisc	0.0000150	Pa×s	907.34	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=R547085&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