

1-Methoxy-2,16-dimethylheptacosane

Inchi:	InChI=1S/C30H62O/c1-5-6-7-8-9-13-16-19-22-25-29(2)26-23-20-17-14-11-10-12-15-18-2
InchiKey:	MWEBQGZVDFKDLN-UHFFFAOYSA-N
Formula:	C30H62O
SMILES:	CCCCCCCCCCCC(C)CCCCCCCCCCCCCCCC(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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001162	Paxs	582.51	Joback Method
dvisc	0.0000577	Paxs	663.72	Joback Method
dvisc	0.0000334	Paxs	744.92	Joback Method
dvisc	0.0000215	Paxs	826.13	Joback Method
dvisc	0.0000150	Paxs	907.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R547114&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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