

1-Methoxy-2,18-dimethylnonacosane

Inchi:	InChI=1S/C32H66O/c1-5-6-7-8-9-15-18-21-24-27-31(2)28-25-22-19-16-13-11-10-12-14-
InchiKey:	XQCKTOZEECCIIR-UHFFFAOYSA-N
Formula:	C32H66O
SMILES:	CCCCCCCCCCCC(C)CCCCCCCCCCCCCCCC(C)COC
Mol. weight [g/mol]:	466.87

Physical Properties

Property code	Value	Unit	Source
gf	108.68	kJ/mol	Joback Method
hf	-846.59	kJ/mol	Joback Method
hfus	72.78	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-11.82		Crippen Method
logp	11.677		Crippen Method
mcvol	467.610	ml/mol	McGowan Method
pc	543.10	kPa	Joback Method
rinpol	3205.00		NIST Webbook
tb	953.10	K	Joback Method
tc	1186.03	K	Joback Method
tf	442.63	K	Joback Method
vc	1.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1655.05	J/molxK	953.10	Joback Method
cpg	1684.04	J/molxK	991.92	Joback Method
cpg	1710.99	J/molxK	1030.74	Joback Method
cpg	1736.00	J/molxK	1069.57	Joback Method
cpg	1759.19	J/molxK	1108.39	Joback Method
cpg	1780.66	J/molxK	1147.21	Joback Method
cpg	1800.53	J/molxK	1186.03	Joback Method
dvisc	0.0007751	Paxs	442.63	Joback Method
dvisc	0.0002149	Paxs	527.71	Joback Method

dvisc	0.0000851	Paxs	612.79	Joback Method
dvisc	0.0000422	Paxs	697.87	Joback Method
dvisc	0.0000244	Paxs	782.94	Joback Method
dvisc	0.0000157	Paxs	868.02	Joback Method
dvisc	0.0000109	Paxs	953.10	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=R547129&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
mccvol:	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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