

1-Methoxy-26-methyloctacosane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C30H62O/c1-4-30(2)28-26-24-22-20-18-16-14-12-10-8-6-5-7-9-11-13-15-17-19

KIRBJEXFCHHLMU-UHFFFAOYSA-N

C30H62O

CCC(C)CCCCCCCCCCCCCCCCCCCCCCCCCOC

438.81

Physical Properties

Property code	Value	Unit	Source
gf	94.28	kJ/mol	Joback Method
hf	-800.03	kJ/mol	Joback Method
hfus	71.12	kJ/mol	Joback Method
hvap	84.40	kJ/mol	Joback Method
log10ws	-11.23		Crippen Method
logp	11.041		Crippen Method
mcvol	439.430	ml/mol	McGowan Method
pc	592.86	kPa	Joback Method
rinpol	3107.00		NIST Webbook
tb	907.78	K	Joback Method
tc	1121.15	K	Joback Method
tf	435.09	K	Joback Method
vc	1.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1518.98	J/mol×K	907.78	Joback Method
cpg	1638.78	J/mol×K	1085.59	Joback Method
cpg	1617.94	J/mol×K	1050.03	Joback Method
cpg	1595.62	J/mol×K	1014.47	Joback Method
cpg	1571.74	J/mol×K	978.90	Joback Method
cpg	1546.22	J/mol×K	943.34	Joback Method
cpg	1658.22	J/mol×K	1121.15	Joback Method
dvisc	0.0000164	Pa×s	907.78	Joback Method
dvisc	0.0000232	Pa×s	829.00	Joback Method

dvisc	0.0000352	Pa×s	750.22	Joback Method
dvisc	0.0000589	Pa×s	671.43	Joback Method
dvisc	0.0001130	Pa×s	592.65	Joback Method
dvisc	0.0002651	Pa×s	513.87	Joback Method
dvisc	0.0008465	Pa×s	435.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R547283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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