

1-Methoxy-2,12-dimethylpentacosane

Inchi:	InChI=1S/C27H56O/c1-5-6-7-8-9-10-11-13-16-19-22-26(2)23-20-17-14-12-15-18-21-24-2
InchiKey:	ZJLHKMKMADAAGX-UHFFFAOYSA-N
Formula:	C27H56O
SMILES:	CCCCCCCCCCCC(C)CCCCCCCC(C)COC
Mol. weight [g/mol]:	396.73

Physical Properties

Property code	Value	Unit	Source
gf	66.58	kJ/mol	Joback Method
hf	-743.39	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.727		Crippen Method
mcvol	397.160	ml/mol	McGowan Method
pc	688.53	kPa	Joback Method
rinpol	2804.00		NIST Webbook
tb	838.70	K	Joback Method
tc	1027.33	K	Joback Method
tf	386.28	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.06	J/molxK	838.70	Joback Method
cpg	1429.39	J/molxK	995.89	Joback Method
cpg	1409.81	J/molxK	964.45	Joback Method
cpg	1389.03	J/molxK	933.01	Joback Method
cpg	1367.01	J/molxK	901.58	Joback Method
cpg	1343.70	J/molxK	870.14	Joback Method
cpg	1447.82	J/molxK	1027.33	Joback Method
dvisc	0.0000237	Paxs	838.70	Joback Method
dvisc	0.0000340	Paxs	763.30	Joback Method

dvisc	0.0000527	Paxs	687.89	Joback Method
dvisc	0.0000909	Paxs	612.49	Joback Method
dvisc	0.0001830	Paxs	537.09	Joback Method
dvisc	0.0004627	Paxs	461.68	Joback Method
dvisc	0.0016806	Paxs	386.28	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=R547050&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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