

1-Methoxy-22-methylpentacosane

Inchi:	InChI=1S/C27H56O/c1-4-24-27(2)25-22-20-18-16-14-12-10-8-6-5-7-9-11-13-15-17-19-21
InchiKey:	PNVHLUPDDVUJQL-UHFFFAOYSA-N
Formula:	C27H56O
SMILES:	CCCC(C)CCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	396.73

Physical Properties

Property code	Value	Unit	Source
gf	69.02	kJ/mol	Joback Method
hf	-738.11	kJ/mol	Joback Method
hfus	63.35	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	9.871		Crippen Method
mvol	397.160	ml/mol	McGowan Method
pc	685.65	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	839.14	K	Joback Method
tc	1028.31	K	Joback Method
tf	401.28	K	Joback Method
vc	1.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.67	J/molxK	839.14	Joback Method
cpg	1343.39	J/molxK	870.67	Joback Method
cpg	1366.77	J/molxK	902.20	Joback Method
cpg	1388.86	J/molxK	933.72	Joback Method
cpg	1409.72	J/molxK	965.25	Joback Method
cpg	1429.38	J/molxK	996.78	Joback Method
cpg	1447.90	J/molxK	1028.31	Joback Method
dvisc	0.0013017	Paxs	401.28	Joback Method

dvisc	0.0004100	Paxs	474.26	Joback Method
dvisc	0.0001758	Paxs	547.23	Joback Method
dvisc	0.0000920	Paxs	620.21	Joback Method
dvisc	0.0000551	Paxs	693.19	Joback Method
dvisc	0.0000365	Paxs	766.16	Joback Method
dvisc	0.0000259	Paxs	839.14	Joback Method

Sources

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=R547238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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