

Docosyl pentyl ether

Inchi:	InChI=1S/C27H56O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27-28
InchiKey:	JQGOHOOIFMOUEK-UHFFFAOYSA-N
Formula:	C27H56O
SMILES:	CCCCCCCCCCCCCCCCCCCCOCCCCC
Mol. weight [g/mol]:	396.73

Physical Properties

Property code	Value	Unit	Source
gf	71.46	kJ/mol	Joback Method
hf	-732.83	kJ/mol	Joback Method
hfus	66.87	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	10.015		Crippen Method
mvol	397.160	ml/mol	McGowan Method
pc	682.78	kPa	Joback Method
rinpol	2775.00		NIST Webbook
tb	839.58	K	Joback Method
tc	1029.43	K	Joback Method
tf	416.28	K	Joback Method
vc	1.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.29	J/molxK	839.58	Joback Method
cpg	1343.10	J/molxK	871.22	Joback Method
cpg	1366.56	J/molxK	902.86	Joback Method
cpg	1388.75	J/molxK	934.50	Joback Method
cpg	1409.69	J/molxK	966.14	Joback Method
cpg	1429.45	J/molxK	997.78	Joback Method
cpg	1448.06	J/molxK	1029.43	Joback Method
dvisc	0.0010370	Paxs	416.28	Joback Method
dvisc	0.0003681	Paxs	486.83	Joback Method

dvisc	0.0001699	Paxs	557.38	Joback Method
dvisc	0.0000933	Paxs	627.93	Joback Method
dvisc	0.0000578	Paxs	698.48	Joback Method
dvisc	0.0000391	Paxs	769.03	Joback Method
dvisc	0.0000282	Paxs	839.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406421&Units=SI
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

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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