

3,11-dimethyl-pentacosane

Inchi:

InChI=1S/C27H56/c1-5-7-8-9-10-11-12-13-14-15-17-21-24-27(4)25-22-19-16-18-20-23-2

InchiKey:

NAGZGURRYTWJLN-UHFFFAOYSA-N

Formula:

C27H56

SMILES:

CCCCCCCCCCCCCCCC(C)CCCCCCCC(C)CC

Mol. weight [g/mol]:

380.73

Physical Properties

Property code	Value	Unit	Source
gf	171.58	kJ/mol	Joback Method
hf	-611.17	kJ/mol	Joback Method
hfus	58.64	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Joback Method
log10ws	-10.64		Crippen Method
logp	10.491		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	694.71	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2607.00		NIST Webbook
rinpol	2604.00		NIST Webbook
rinpol	2609.00		NIST Webbook
rinpol	2608.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	816.28	K	Joback Method
tc	999.37	K	Joback Method
tf	364.05	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.57	J/mol×K	816.28	Joback Method
cpg	1307.23	J/mol×K	846.80	Joback Method
cpg	1330.65	J/mol×K	877.31	Joback Method

cpg	1352.88	J/mol×K	907.83	Joback Method
cpg	1373.98	J/mol×K	938.34	Joback Method
cpg	1394.00	J/mol×K	968.86	Joback Method
cpg	1412.98	J/mol×K	999.37	Joback Method
dvisc	0.0027479	Pa×s	364.05	Joback Method
dvisc	0.0006915	Pa×s	439.42	Joback Method
dvisc	0.0002606	Pa×s	514.79	Joback Method
dvisc	0.0001260	Pa×s	590.16	Joback Method
dvisc	0.0000719	Pa×s	665.54	Joback Method
dvisc	0.0000459	Pa×s	740.91	Joback Method
dvisc	0.0000319	Pa×s	816.28	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=R261959&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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