

3,13-dimethyl-pentacosane

Other names:	Pentacosane, 3,13-dimethyl
Inchi:	InChI=1S/C27H56/c1-5-7-8-9-10-11-12-14-18-21-24-27(4)25-22-19-16-13-15-17-20-23-2
InchiKey:	QVYBPDSFHVRTOG-UHFFFAOYSA-N
Formula:	C27H56
SMILES:	CCCCCCCCCCCCC(C)CCCCCCCCC(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	2604.00		NIST Webbook
rinpol	2608.00		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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R404552&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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