

6,9,12,15-Nonacosatetraene

Inchi:	InChI=1S/C29H52/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-28-26-24-22-20-18-16-14-
InchiKey:	BFWBDNQAJZQPIB-WVKOCGEKSA-N
Formula:	C29H52
SMILES:	CCCCC=CCC=CCC=CCC=CCCCCCCCCCCCC
Mol. weight [g/mol]:	400.72

Physical Properties

Property code	Value	Unit	Source
gf	514.18	kJ/mol	Joback Method
hf	-173.01	kJ/mol	Joback Method
hfus	71.67	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-11.38		Crippen Method
logp	10.663		Crippen Method
mcvol	402.270	ml/mol	McGowan Method
pc	694.71	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	879.56	K	Joback Method
tc	1076.91	K	Joback Method
tf	396.27	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.57	J/molxK	879.56	Joback Method
cpg	1335.07	J/molxK	912.45	Joback Method
cpg	1357.60	J/molxK	945.34	Joback Method
cpg	1379.24	J/molxK	978.24	Joback Method
cpg	1400.13	J/molxK	1011.13	Joback Method
cpg	1420.36	J/molxK	1044.02	Joback Method
cpg	1440.05	J/molxK	1076.91	Joback Method

dvisc	0.0009787	Paxs	396.27	Joback Method
dvisc	0.0002788	Paxs	476.82	Joback Method
dvisc	0.0001141	Paxs	557.37	Joback Method
dvisc	0.0000586	Paxs	637.91	Joback Method
dvisc	0.0000349	Paxs	718.46	Joback Method
dvisc	0.0000231	Paxs	799.01	Joback Method
dvisc	0.0000165	Paxs	879.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R627082&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
mvol:	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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