

5,9-dimethylnonacosane

Other names:	Nonacosane, 5,9-dimethyl
Inchi:	InChI=1S/C31H64/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-27-31(4)29
InchiKey:	HALZPFCKYZKALP-UHFFFAOYSA-N
Formula:	C31H64
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC
Mol. weight [g/mol]:	436.84

Physical Properties

Property code	Value	Unit	Source
gf	205.26	kJ/mol	Joback Method
hf	-693.73	kJ/mol	Joback Method
hfus	69.00	kJ/mol	Joback Method
hvap	83.82	kJ/mol	Joback Method
log10ws	-12.32		Crippen Method
logp	12.051		Crippen Method
mcvol	447.650	ml/mol	McGowan Method
pc	572.88	kPa	Joback Method
rinpol	2983.00		NIST Webbook
rinpol	2982.00		NIST Webbook
rinpol	2983.00		NIST Webbook
rinpol	2982.00		NIST Webbook
rinpol	2976.00		NIST Webbook
tb	907.80	K	Joback Method
tc	1120.00	K	Joback Method
tf	409.13	K	Joback Method
vc	1.760	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1550.48	J/mol×K	907.80	Joback Method
cpg	1674.29	J/mol×K	1084.64	Joback Method
cpg	1652.45	J/mol×K	1049.27	Joback Method
cpg	1629.24	J/mol×K	1013.90	Joback Method

cpg	1604.57	J/mol×K	978.53	Joback Method
cpg	1578.35	J/mol×K	943.17	Joback Method
cpg	1694.85	J/mol×K	1120.00	Joback Method
dvisc	0.0000174	Paxs	907.80	Joback Method
dvisc	0.0000251	Paxs	824.69	Joback Method
dvisc	0.0000394	Paxs	741.58	Joback Method
dvisc	0.0000691	Paxs	658.46	Joback Method
dvisc	0.0001427	Paxs	575.35	Joback Method
dvisc	0.0003763	Paxs	492.24	Joback Method
dvisc	0.0014719	Paxs	409.13	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=R195278&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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