

9,13-dimethylnonacosane

Inchi:	InChI=1S/C31H64/c1-5-7-9-11-13-14-15-16-17-18-19-20-22-24-27-31(4)29-25-28-30(3)2
InchiKey:	IHFOKUGZVRWBAV-UHFFFAOYSA-N
Formula:	C31H64
SMILES:	CCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCC
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
mvol	447.650	ml/mol	McGowan Method
pc	572.88	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2963.00		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/molxK	907.80	Joback Method
cpg	1578.35	J/molxK	943.17	Joback Method
cpg	1604.57	J/molxK	978.53	Joback Method
cpg	1629.24	J/molxK	1013.90	Joback Method
cpg	1652.45	J/molxK	1049.27	Joback Method
cpg	1674.29	J/molxK	1084.64	Joback Method
cpg	1694.85	J/molxK	1120.00	Joback Method
dvisc	0.0014719	Paxs	409.13	Joback Method

dvisc	0.0003763	Paxs	492.24	Joback Method
dvisc	0.0001427	Paxs	575.35	Joback Method
dvisc	0.0000691	Paxs	658.46	Joback Method
dvisc	0.0000394	Paxs	741.58	Joback Method
dvisc	0.0000251	Paxs	824.69	Joback Method
dvisc	0.0000174	Paxs	907.80	Joback Method

Sources

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=R262229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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