

3,9-dimethyl-nonacosane

Inchi: InChI=1S/C31H64/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-28-31(4)29-2
InchiKey: NDOVDOYSHIGRRI-UHFFFAOYSA-N
Formula: C31H64
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCCC(C)CC
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	3001.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3007.00		NIST Webbook
rinpol	3006.00		NIST Webbook
tb	907.80	K	Joback Method
tc	1120.00	K	Joback Method
tf	409.13	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1550.48	J/mol×K	907.80	Joback Method
cpg	1578.35	J/mol×K	943.17	Joback Method
cpg	1604.57	J/mol×K	978.53	Joback Method
cpg	1629.24	J/mol×K	1013.90	Joback Method

cpg	1652.45	J/mol×K	1049.27	Joback Method
cpg	1674.29	J/mol×K	1084.64	Joback Method
cpg	1694.85	J/mol×K	1120.00	Joback Method
dvisc	0.0014719	Pa×s	409.13	Joback Method
dvisc	0.0003763	Pa×s	492.24	Joback Method
dvisc	0.0001427	Pa×s	575.35	Joback Method
dvisc	0.0000691	Pa×s	658.46	Joback Method
dvisc	0.0000394	Pa×s	741.58	Joback Method
dvisc	0.0000251	Pa×s	824.69	Joback Method
dvisc	0.0000174	Pa×s	907.80	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=R262036&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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