3,13-dimethyl-nonacosane

Inchi: InChI=1S/C31H64/c1-5-7-8-9-10-11-12-13-14-15-16-18-22-25-28-31(4)29-26-23-20-17-1
InchiKey: PBHGXRCCYYTOAK-UHFFFAOYSA-N
Formula: C31H64
SMILES: CCCCCCCCCCCCCCCCC(C)CCCCCCCCCC(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	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3001.00		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	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	Pa×s	907.80	Joback Method
dvisc	0.0000251	Pa×s	824.69	Joback Method
dvisc	0.0000394	Pa×s	741.58	Joback Method
dvisc	0.0000691	Pa×s	658.46	Joback Method
dvisc	0.0001427	Pa×s	575.35	Joback Method
dvisc	0.0003763	Pa×s	492.24	Joback Method
dvisc	0.0014719	Pa×s	409.13	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=R404547&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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