Nonacosane, 5,19-dimethyl

Inchi: InChI=1S/C31H64/c1-5-7-9-10-11-17-20-24-28-31(4)29-25-22-19-16-14-12-13-15-18-21-
InchiKey: RTGCYNHFNNPTDB-UHFFFAOYSA-N
Formula: C31H64
SMILES: CCCCCCCCCCC(C)CCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 436.85

Physical Properties

Property code	Value	Unit	Source
af	1.1595		Cheméo Relay (1.0)
gf	205.26	kJ/mol	Joback Method
hf	-720.63	kJ/mol	Cheméo Relay (1.0)
hfus	69.00	kJ/mol	Joback Method
hvap	145.18	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-11.48		Cheméo Relay (1.0)
logp	12.051		Crippen Method
mcvol	447.650	ml/mol	McGowan Method
pc	572.88	kPa	Joback Method
rinpol	2983.00		NIST Webbook
rinpol	2983.00		NIST Webbook
rinpol	2983.00		NIST Webbook
tb	646.35	K	Cheméo Relay (1.0)
tc	818.28	K	Cheméo Relay (1.0)
tf	286.69	K	Cheméo Relay (1.0)
vc	1.749	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R505630&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
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