1-Nonacosene

Inchi: InChI=1S/C29H58/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-28-26-24-22-20-18-16-14-

InchiKey: UBMJSQAFNUWJEG-UHFFFAOYSA-N

Formula: C29H52

SMILES: C=CCCCCCCCCCCCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 400.72

CAS: 18835-35-3

Physical Properties

Property code	Value	Unit	Source
gf	281.14	kJ/mol	Joback Method
hf	-516.46	kJ/mol	Joback Method
hfus	69.59	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-11.82		Crippen Method
logp	11.335		Crippen Method
mcvol	415.170	ml/mol	McGowan Method
pc	637.69	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2877.00		NIST Webbook
rinpol	2888.00		NIST Webbook
rinpol	2884.70		NIST Webbook
tb	859.60	K	Joback Method
tc	1055.27	K	Joback Method
tf	414.83	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.92	J/mol×K	859.60	Joback Method
cpg	1411.53	J/mol×K	892.21	Joback Method
cpg	1435.79	J/mol×K	924.82	Joback Method
cpg	1458.77	J/mol×K	957.43	Joback Method
cpg	1480.54	J/mol×K	990.05	Joback Method

cpg	1501.18	J/mol×K	1022.66	Joback Method
cpg	1520.75	J/mol×K	1055.27	Joback Method
dvisc	0.0012385	Pa×s	414.83	Joback Method
dvisc	0.0004174	Pa×s	488.96	Joback Method
dvisc	0.0001873	Pa×s	563.09	Joback Method
dvisc	0.0001013	Pa×s	637.22	Joback Method
dvisc	0.0000623	Pa×s	711.34	Joback Method
dvisc	0.0000420	Pa×s	785.47	Joback Method
dvisc	0.0000303	Pa×s	859.60	Joback Method
hvapt	113.30	kJ/mol	584.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.16621e+01
Coeff. B	-3.16266e+03
Coeff. C	-2.61912e+02
Temperature range (K), min.	539.96
Temperature range (K), max.	759.92

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18835353&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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