

2-Methylnonacosane

Other names:	Nonacosane, 2-methyl-
Inchi:	InChI=1S/C30H62/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey:	NLAGNNORBYGNAV-UHFFFAOYSA-N
Formula:	C30H62
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]:	422.81
CAS:	1560-75-4

Physical Properties

Property code	Value	Unit	Source
gf	199.28	kJ/mol	Joback Method
hf	-667.81	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	81.99	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	11.805		Crippen Method
mcvol	433.560	ml/mol	McGowan Method
pc	597.80	kPa	Joback Method
rinpol	2960.60		NIST Webbook
rinpol	2958.00		NIST Webbook
rinpol	2962.00		NIST Webbook
rinpol	2965.00		NIST Webbook
rinpol	2965.70		NIST Webbook
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
rinpol	2958.00		NIST Webbook
tb	885.36	K	Joback Method
tc	1090.03	K	Joback Method
tf	412.86	K	Joback Method
vc	1.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	1623.76	J/mol×K	1090.03	Joback Method
cpg	1603.48	J/mol×K	1055.92	Joback Method
cpg	1582.00	J/mol×K	1021.80	Joback Method
cpg	1559.23	J/mol×K	987.69	Joback Method
cpg	1535.09	J/mol×K	953.58	Joback Method
cpg	1509.50	J/mol×K	919.47	Joback Method
cpg	1482.38	J/mol×K	885.36	Joback Method
dvisc	0.0013422	Pa×s	412.86	Joback Method
dvisc	0.0000222	Pa×s	885.36	Joback Method
dvisc	0.0000315	Pa×s	806.61	Joback Method
dvisc	0.0000482	Pa×s	727.86	Joback Method
dvisc	0.0000818	Pa×s	649.11	Joback Method
dvisc	0.0001607	Pa×s	570.36	Joback Method
dvisc	0.0003919	Pa×s	491.61	Joback Method
hvapt	116.80	kJ/mol	589.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1560754&Units=SI

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
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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