

17,21-dimethylnonatriacontane

Inchi:	InChI=1S/C41H84/c1-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-37-41(4)39-35-38
InchiKey:	YFTTUSZBCPWOLF-UHFFFAOYSA-N
Formula:	C41H84
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	577.11

Physical Properties

Property code	Value	Unit	Source
gf	289.46	kJ/mol	Joback Method
hf	-900.13	kJ/mol	Joback Method
hfus	94.90	kJ/mol	Joback Method
hvap	106.08	kJ/mol	Joback Method
log10ws	-16.50		Crippen Method
logp	15.952		Crippen Method
mcvol	588.550	ml/mol	McGowan Method
pc	378.80	kPa	Joback Method
rinpol	3955.00		NIST Webbook
rinpol	3955.00		NIST Webbook
rinpol	3955.00		NIST Webbook
tb	1136.60	K	Joback Method
tc	1525.89	K	Joback Method
tf	521.83	K	Joback Method
vc	2.320	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2246.73	J/mol×K	1136.60	Joback Method
cpg	2435.56	J/mol×K	1461.01	Joback Method
cpg	2403.06	J/mol×K	1396.13	Joback Method
cpg	2368.72	J/mol×K	1331.25	Joback Method
cpg	2331.73	J/mol×K	1266.36	Joback Method
cpg	2291.33	J/mol×K	1201.48	Joback Method
cpg	2466.97	J/mol×K	1525.89	Joback Method

dvisc	0.0000035	Paxs	1136.60	Joback Method
dvisc	0.0000050	Paxs	1034.14	Joback Method
dvisc	0.0000079	Paxs	931.68	Joback Method
dvisc	0.0000138	Paxs	829.21	Joback Method
dvisc	0.0000284	Paxs	726.75	Joback Method
dvisc	0.0000742	Paxs	624.29	Joback Method
dvisc	0.0002822	Paxs	521.83	Joback Method

Sources

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=R272241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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