

7,13-Dimethylnonatriacontane

Inchi: InChI=1S/C41H84/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41
InchiKey: PQICEKZMTWQGFGQ-UHFFFAOYSA-N
Formula: C41H84
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCCC
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
mvol	588.550	ml/mol	McGowan Method
pc	378.80	kPa	Joback Method
rinpol	3853.00		NIST Webbook
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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/molxK	1136.60	Joback Method
cpg	2435.56	J/molxK	1461.01	Joback Method
cpg	2403.06	J/molxK	1396.13	Joback Method
cpg	2368.72	J/molxK	1331.25	Joback Method
cpg	2331.73	J/molxK	1266.36	Joback Method
cpg	2291.33	J/molxK	1201.48	Joback Method
cpg	2466.97	J/molxK	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R539430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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