

9,13,19-trimethylnonatriacontane

Inchi:	InChI=1S/C42H86/c1-6-8-10-12-14-15-16-17-18-19-20-21-22-23-24-25-27-30-34-40(3)36
InchiKey:	PXJGSMKRFGWFJE-UHFFFAOYSA-N
Formula:	C42H86
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCC
Mol. weight [g/mol]:	591.13

Physical Properties

Property code	Value	Unit	Source
gf	295.44	kJ/mol	Joback Method
hf	-926.05	kJ/mol	Joback Method
hfus	93.97	kJ/mol	Joback Method
hvap	107.92	kJ/mol	Joback Method
log10ws	-16.68		Crippen Method
logp	16.198		Crippen Method
mvol	602.640	ml/mol	McGowan Method
pc	366.15	kPa	Joback Method
rinpol	3970.00		NIST Webbook
rinpol	3970.00		NIST Webbook
tb	1159.04	K	Joback Method
tc	1569.41	K	Joback Method
tf	518.10	K	Joback Method
vc	2.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.43	J/molxK	1159.04	Joback Method
cpg	2363.53	J/molxK	1227.44	Joback Method
cpg	2405.17	J/molxK	1295.83	Joback Method
cpg	2443.29	J/molxK	1364.23	Joback Method
cpg	2478.81	J/molxK	1432.62	Joback Method
cpg	2512.67	J/molxK	1501.02	Joback Method
cpg	2545.81	J/molxK	1569.41	Joback Method
dvisc	0.0002834	Paxs	518.10	Joback Method

dvisc	0.0000668	Paxs	624.92	Joback Method
dvisc	0.0000240	Paxs	731.75	Joback Method
dvisc	0.0000112	Paxs	838.57	Joback Method
dvisc	0.0000062	Paxs	945.39	Joback Method
dvisc	0.0000039	Paxs	1052.22	Joback Method
dvisc	0.0000026	Paxs	1159.04	Joback Method

Sources

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=R280712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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