

9,13,21-trimethyltrtriacontane

Inchi:	InChI=1S/C36H74/c1-6-8-10-12-14-15-16-17-20-24-28-34(3)29-25-21-18-22-26-31-36(5)
InchiKey:	LITSHDBRQYPISW-UHFFFAOYSA-N
Formula:	C36H74
SMILES:	CCCCCCCCCCCC(C)CCCCCCCC(C)CCCC(C)CCCCCCCC
Mol. weight [g/mol]:	506.97

Physical Properties

Property code	Value	Unit	Source
gf	244.92	kJ/mol	Joback Method
hf	-802.21	kJ/mol	Joback Method
hfus	78.43	kJ/mol	Joback Method
hvap	94.57	kJ/mol	Joback Method
log10ws	-14.17		Crippen Method
logp	13.857		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	462.48	kPa	Joback Method
rinpol	3380.00		NIST Webbook
rinpol	3385.00		NIST Webbook
tb	1021.76	K	Joback Method
tc	1294.81	K	Joback Method
tf	450.48	K	Joback Method
vc	2.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.31	J/molxK	1021.76	Joback Method
cpg	2040.85	J/molxK	1249.30	Joback Method
cpg	2015.88	J/molxK	1203.80	Joback Method
cpg	1989.08	J/molxK	1158.29	Joback Method
cpg	1960.20	J/molxK	1112.78	Joback Method
cpg	1929.03	J/molxK	1067.27	Joback Method
cpg	2064.22	J/molxK	1294.81	Joback Method
dvisc	0.0000072	Paxs	1021.76	Joback Method

dvisc	0.0000105	Paxs	926.55	Joback Method
dvisc	0.0000168	Paxs	831.33	Joback Method
dvisc	0.0000305	Paxs	736.12	Joback Method
dvisc	0.0000658	Paxs	640.91	Joback Method
dvisc	0.0001858	Paxs	545.69	Joback Method
dvisc	0.0008138	Paxs	450.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R272776&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

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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