

13-methylnonatriacontane

Inchi:	InChI=1S/C40H82/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-23-24-25-26-27-28-29-31-33
InchiKey:	KSCNZEGERKUME-UHFFFAOYSA-N
Formula:	C40H82
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	563.08

Physical Properties

Property code	Value	Unit	Source
gf	283.48	kJ/mol	Joback Method
hf	-874.21	kJ/mol	Joback Method
hfus	95.83	kJ/mol	Joback Method
hvap	104.25	kJ/mol	Joback Method
log10ws	-16.32		Crippen Method
logp	15.706		Crippen Method
mcvol	574.460	ml/mol	McGowan Method
pc	392.12	kPa	Joback Method
rinpola	3920.00		NIST Webbook
tb	1114.16	K	Joback Method
tc	1483.64	K	Joback Method
tf	525.56	K	Joback Method
vc	2.269	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2176.07	J/molxK	1114.16	Joback Method
cpg	2219.21	J/molxK	1175.74	Joback Method
cpg	2258.42	J/molxK	1237.32	Joback Method
cpg	2294.36	J/molxK	1298.90	Joback Method
cpg	2327.67	J/molxK	1360.48	Joback Method
cpg	2359.01	J/molxK	1422.06	Joback Method
cpg	2389.02	J/molxK	1483.64	Joback Method
dvisc	0.0002820	Paxs	525.56	Joback Method
dvisc	0.0000823	Paxs	623.66	Joback Method

dvisc	0.0000336	Paxs	721.76	Joback Method
dvisc	0.0000170	Paxs	819.86	Joback Method
dvisc	0.0000099	Paxs	917.96	Joback Method
dvisc	0.0000064	Paxs	1016.06	Joback Method
dvisc	0.0000045	Paxs	1114.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280103&Units=SI
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

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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