

21-methylhentetracontane

Inchi:	InChI=1S/C42H86/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36-38-40-42(3)41-
InchiKey:	JJPCBMIUAYWSEL-UHFFFAOYSA-N
Formula:	C42H86
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	591.13

Physical Properties

Property code	Value	Unit	Source
gf	300.32	kJ/mol	Joback Method
hf	-915.49	kJ/mol	Joback Method
hfus	101.01	kJ/mol	Joback Method
hvap	108.70	kJ/mol	Joback Method
log10ws	-17.16		Crippen Method
logp	16.486		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	363.92	kPa	Joback Method
rinpola	4113.00		NIST Webbook
tb	1159.92	K	Joback Method
tc	1588.64	K	Joback Method
tf	548.10	K	Joback Method
vc	2.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.86	J/molxK	1159.92	Joback Method
cpg	2366.40	J/molxK	1231.37	Joback Method
cpg	2410.23	J/molxK	1302.83	Joback Method
cpg	2450.42	J/molxK	1374.28	Joback Method
cpg	2488.04	J/molxK	1445.73	Joback Method
cpg	2524.16	J/molxK	1517.18	Joback Method
cpg	2559.84	J/molxK	1588.64	Joback Method
dvisc	0.0002032	Paxs	548.10	Joback Method
dvisc	0.0000593	Paxs	650.07	Joback Method

dvisc	0.0000242	Paxs	752.04	Joback Method
dvisc	0.0000122	Paxs	854.01	Joback Method
dvisc	0.0000071	Paxs	955.98	Joback Method
dvisc	0.0000046	Paxs	1057.95	Joback Method
dvisc	0.0000032	Paxs	1159.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280163&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

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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