

13,17,21,25-Tetramethylheptatriacontane

Inchi:	InChI=1S/C42H86/c1-7-9-11-13-15-17-19-21-23-25-27-32-40(4)34-29-36-42(6)38-30-37
InchiKey:	YJNXZHUQBSZRBH-UHFFFAOYSA-N
Formula:	C42H86
SMILES:	CCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	591.13

Physical Properties

Property code	Value	Unit	Source
gf	293.00	kJ/mol	Joback Method
hf	-931.33	kJ/mol	Joback Method
hfus	90.44	kJ/mol	Joback Method
hvap	107.53	kJ/mol	Joback Method
log10ws	-16.44		Crippen Method
logp	16.054		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	367.28	kPa	Joback Method
rinpol	3807.00		NIST Webbook
tb	1158.60	K	Joback Method
tc	1560.30	K	Joback Method
tf	503.10	K	Joback Method
vc	2.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.22	J/molxK	1158.60	Joback Method
cpg	2362.17	J/molxK	1225.55	Joback Method
cpg	2402.78	J/molxK	1292.50	Joback Method
cpg	2439.92	J/molxK	1359.45	Joback Method
cpg	2474.46	J/molxK	1426.40	Joback Method
cpg	2507.29	J/molxK	1493.35	Joback Method
cpg	2539.27	J/molxK	1560.30	Joback Method
dvisc	0.0003438	Paxs	503.10	Joback Method
dvisc	0.0000718	Paxs	612.35	Joback Method

dvisc	0.0000241	Paxs	721.60	Joback Method
dvisc	0.0000108	Paxs	830.85	Joback Method
dvisc	0.0000058	Paxs	940.10	Joback Method
dvisc	0.0000036	Paxs	1049.35	Joback Method
dvisc	0.0000024	Paxs	1158.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337501&Units=SI

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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