6,10,24,28-tetramethyloctatriacontane

Inchi: InChI=1S/C42H86/c1-7-9-11-12-13-19-22-26-32-41(5)37-30-38-42(6)34-28-24-21-18-16-
InchiKey: KBDUHTOBAJJICC-UHFFFAOYSA-N
Formula: C42H86
SMILES: CCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCC(C)CCCC(C)CCCCC
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	3915.00		NIST Webbook
rinpol	3915.00		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/mol×K	1158.60	Joback Method
cpg	2362.17	J/mol×K	1225.55	Joback Method
cpg	2402.78	J/mol×K	1292.50	Joback Method
cpg	2439.92	J/mol×K	1359.45	Joback Method
cpg	2474.46	J/mol×K	1426.40	Joback Method
cpg	2507.29	J/mol×K	1493.35	Joback Method
cpg	2539.27	J/mol×K	1560.30	Joback Method
dvisc	0.0003438	Pa×s	503.10	Joback Method

dvisc	0.0000718	Pa×s	612.35	Joback Method
dvisc	0.0000241	Pa×s	721.60	Joback Method
dvisc	0.0000108	Pa×s	830.85	Joback Method
dvisc	0.0000058	Pa×s	940.10	Joback Method
dvisc	0.0000036	Pa×s	1049.35	Joback Method
dvisc	0.0000024	Pa×s	1158.60	Joback Method

Sources

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=R280450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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