7,11,21-trimethylhentetracontane

Inchi: InChI=1S/C44H90/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-23-25-28-32-37-42(3)38
InchiKey: JBWGFNKILBTEDD-UHFFFAOYSA-N
Formula: C44H90
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCC(C)CCCC(C)CCCCCC
Mol. weight [g/mol]: 619.19

Physical Properties

Property code	Value	Unit	Source
gf	312.28	kJ/mol	Joback Method
hf	-967.33	kJ/mol	Joback Method
hfus	99.15	kJ/mol	Joback Method
hvap	112.37	kJ/mol	Joback Method
log10ws	-17.52		Crippen Method
logp	16.978		Crippen Method
mcvol	630.820	ml/mol	McGowan Method
pc	340.66	kPa	Joback Method
rinpol	4177.00		NIST Webbook
tb	1204.80	K	Joback Method
tc	1682.83	K	Joback Method
tf	540.64	K	Joback Method
vc	2.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2459.60	J/mol×K	1204.80	Joback Method
cpg	2511.69	J/mol×K	1284.47	Joback Method
cpg	2558.56	J/mol×K	1364.14	Joback Method
cpg	2601.77	J/mol×K	1443.82	Joback Method
cpg	2642.87	J/mol×K	1523.49	Joback Method
cpg	2683.40	J/mol×K	1603.16	Joback Method
cpg	2724.92	J/mol×K	1682.83	Joback Method
dvisc	0.0001986	Pa×s	540.64	Joback Method
dvisc	0.0000473	Pa×s	651.33	Joback Method

dvisc	0.0000171	Pa×s	762.03	Joback Method
dvisc	0.0000080	Pa×s	872.72	Joback Method
dvisc	0.0000044	Pa×s	983.41	Joback Method
dvisc	0.0000028	Pa×s	1094.11	Joback Method
dvisc	0.0000019	Pa×s	1204.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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