

5,9,13,21-tetramethylnonatriacontane

Inchi: InChI=1S/C43H88/c1-7-9-11-12-13-14-15-16-17-18-19-20-21-22-24-27-33-41(4)34-28-25
InchiKey: ATCCMNVIWKSXTB-UHFFFAOYSA-N
Formula: C43H88
SMILES: CCCCCCCCCCCCCCCCCC(C)CCCCCCCC(C)CCCC(C)CCCC(C)CCCC
Mol. weight [g/mol]: 605.16

Physical Properties

Property code	Value	Unit	Source
gf	301.42	kJ/mol	Joback Method
hf	-951.97	kJ/mol	Joback Method
hfus	93.03	kJ/mol	Joback Method
hvap	109.76	kJ/mol	Joback Method
log10ws	-16.86		Crippen Method
logp	16.444		Crippen Method
mcvol	616.730	ml/mol	McGowan Method
pc	354.13	kPa	Joback Method
rinpol	4031.00		NIST Webbook
tb	1181.48	K	Joback Method
tc	1614.28	K	Joback Method
tf	514.37	K	Joback Method
vc	2.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2388.15	J/mol×K	1181.48	Joback Method
cpg	2435.81	J/mol×K	1253.61	Joback Method
cpg	2478.75	J/mol×K	1325.75	Joback Method
cpg	2518.10	J/mol×K	1397.88	Joback Method
cpg	2554.97	J/mol×K	1470.01	Joback Method
cpg	2590.50	J/mol×K	1542.15	Joback Method
cpg	2625.79	J/mol×K	1614.28	Joback Method
dvisc	0.0002858	Pa×s	514.37	Joback Method
dvisc	0.0000601	Pa×s	625.55	Joback Method

dvisc	0.0000203	Pa×s	736.74	Joback Method
dvisc	0.0000091	Pa×s	847.92	Joback Method
dvisc	0.0000049	Pa×s	959.11	Joback Method
dvisc	0.0000030	Pa×s	1070.30	Joback Method
dvisc	0.0000020	Pa×s	1181.48	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=R280287&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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