

Hentriacontane, 2,6,10,14,18,22,26,30-octamethyl

Inchi: InChI=1S/C39H80/c1-32(2)18-11-20-34(5)22-13-24-36(7)26-15-28-38(9)30-17-31-39(10)
InchiKey: NYHGCTVGEQJTB-UHFFFAOYSA-N
Formula: C39H80
SMILES: CC(C)CCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 549.05

Physical Properties

Property code	Value	Unit	Source
gf	257.98	kJ/mol	Joback Method
hf	-890.53	kJ/mol	Joback Method
hfus	68.58	kJ/mol	Joback Method
hvap	99.30	kJ/mol	Joback Method
log10ws	-14.21		Crippen Method
logp	14.307		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	416.83	kPa	Joback Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
tb	1088.20	K	Joback Method
tc	1391.58	K	Joback Method
tf	409.29	K	Joback Method
vc	2.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.45	J/molxK	1088.20	Joback Method
cpg	2255.10	J/molxK	1341.02	Joback Method
cpg	2229.81	J/molxK	1290.46	Joback Method
cpg	2202.55	J/molxK	1239.89	Joback Method
cpg	2172.97	J/molxK	1189.33	Joback Method

cpg	2140.72	J/molxK	1138.76	Joback Method
cpg	2278.77	J/molxK	1391.58	Joback Method
dvisc	0.0000027	Paxs	1088.20	Joback Method
dvisc	0.0000042	Paxs	975.05	Joback Method
dvisc	0.0000075	Paxs	861.90	Joback Method
dvisc	0.0000160	Paxs	748.74	Joback Method
dvisc	0.0000443	Paxs	635.59	Joback Method
dvisc	0.0001908	Paxs	522.44	Joback Method
dvisc	0.0018421	Paxs	409.29	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=R213777&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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