

5-Methylhentriacontane

Other names: Hentriacontane, 5-methyl-
Inchi: InChI=1S/C32H66/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32
InchiKey: LRFHJFYLGVEQSB-UHFFFAOYSA-N
Formula: C32H66
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 450.87

Physical Properties

Property code	Value	Unit	Source
gf	216.12	kJ/mol	Joback Method
hf	-709.09	kJ/mol	Joback Method
hfus	75.11	kJ/mol	Joback Method
hvap	86.44	kJ/mol	Joback Method
log10ws	-12.98		Crippen Method
logp	12.585		Crippen Method
mcvol	461.740	ml/mol	McGowan Method
pc	545.39	kPa	Joback Method
rinpol	3145.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3149.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3152.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	931.12	K	Joback Method
tc	1155.67	K	Joback Method
tf	435.40	K	Joback Method
vc	1.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.39	J/molxK	931.12	Joback Method
cpg	1647.62	J/molxK	968.55	Joback Method
cpg	1675.03	J/molxK	1005.97	Joback Method
cpg	1700.75	J/molxK	1043.40	Joback Method
cpg	1724.89	J/molxK	1080.82	Joback Method
cpg	1747.56	J/molxK	1118.25	Joback Method
cpg	1768.88	J/molxK	1155.67	Joback Method
dvisc	0.0009952	Paxs	435.40	Joback Method
dvisc	0.0002905	Paxs	518.02	Joback Method
dvisc	0.0001190	Paxs	600.64	Joback Method
dvisc	0.0000605	Paxs	683.26	Joback Method
dvisc	0.0000356	Paxs	765.88	Joback Method
dvisc	0.0000232	Paxs	848.50	Joback Method
dvisc	0.0000163	Paxs	931.12	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=R203740&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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