

Hexadecane, 3-pentyl

Inchi:	InChI=1S/C21H44/c1-4-7-9-10-11-12-13-14-15-16-18-20-21(6-3)19-17-8-5-2/h21H,4-20H
InchiKey:	QRLUEOCYONDNRP-UHFFFAOYSA-N
Formula:	C21H44
SMILES:	CCCCCCCCCCCCC(CC)CCCC
Mol. weight [g/mol]:	296.57

Physical Properties

Property code	Value	Unit	Source
gf	123.50	kJ/mol	Joback Method
hf	-482.05	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	61.95	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	679.44	K	Joback Method
tc	842.66	K	Joback Method
tf	311.43	K	Joback Method
vc	1.206	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.08	J/molxK	679.44	Joback Method
cpg	922.65	J/molxK	706.64	Joback Method
cpg	943.32	J/molxK	733.85	Joback Method
cpg	963.10	J/molxK	761.05	Joback Method
cpg	982.02	J/molxK	788.26	Joback Method
cpg	1000.12	J/molxK	815.46	Joback Method
cpg	1017.42	J/molxK	842.66	Joback Method
dvisc	0.0045387	Paxs	311.43	Joback Method

dvisc	0.0013283	Paxs	372.76	Joback Method
dvisc	0.0005501	Paxs	434.10	Joback Method
dvisc	0.0002834	Paxs	495.44	Joback Method
dvisc	0.0001690	Paxs	556.77	Joback Method
dvisc	0.0001116	Paxs	618.11	Joback Method
dvisc	0.0000795	Paxs	679.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47661&Units=SI
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

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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