Hexadecane, 7-pentyl

Inchi: InChI=1S/C21H44/c1-4-7-10-12-13-14-17-20-21(18-15-9-6-3)19-16-11-8-5-2/h21H,4-20H
InchiKey: DTFOICPZUYKVTG-UHFFFAOYSA-N
Formula: C21H44
SMILES: CCCCCCCCCC(CCCCC)CCCCCC
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	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook
tb	679.44	K	Joback Method
tc	842.66	K	Joback Method
tf	311.43	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.08	J/mol×K	679.44	Joback Method
cpg	922.65	J/mol×K	706.64	Joback Method
cpg	943.32	J/mol×K	733.85	Joback Method
cpg	963.10	J/mol×K	761.05	Joback Method
cpg	982.02	J/mol×K	788.26	Joback Method
cpg	1000.12	J/mol×K	815.46	Joback Method

cpg	1017.42	J/mol×K	842.66	Joback Method
dvisc	0.0045387	Pa×s	311.43	Joback Method
dvisc	0.0013283	Pa×s	372.76	Joback Method
dvisc	0.0005501	Pa×s	434.10	Joback Method
dvisc	0.0002834	Pa×s	495.44	Joback Method
dvisc	0.0001690	Pa×s	556.77	Joback Method
dvisc	0.0001116	Pa×s	618.11	Joback Method
dvisc	0.0000795	Pa×s	679.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R8761&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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