Hexadecane, 7-hexyl

Inchi: InChI=1S/C22H46/c1-4-7-10-13-14-15-18-21-22(19-16-11-8-5-2)20-17-12-9-6-3/h22H,4-
InchiKey: WRACLUKIERBDNK-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCCC(CCCCCC)CCCCCC
Mol. weight [g/mol]: 310.60

Physical Properties

Property code	Value	Unit	Source
gf	131.92	kJ/mol	Joback Method
hf	-502.69	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	702.32	K	Joback Method
tc	867.26	K	Joback Method
tf	322.70	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.39	J/mol×K	702.32	Joback Method
cpg	984.38	J/mol×K	729.81	Joback Method
cpg	1005.42	J/mol×K	757.30	Joback Method
cpg	1025.55	J/mol×K	784.79	Joback Method
cpg	1044.78	J/mol×K	812.28	Joback Method
cpg	1063.16	J/mol×K	839.77	Joback Method
cpg	1080.72	J/mol×K	867.26	Joback Method
dvisc	0.0040182	Pa×s	322.70	Joback Method

dvisc	0.0011754	Pa×s	385.97	Joback Method
dvisc	0.0004861	Pa×s	449.24	Joback Method
dvisc	0.0002500	Pa×s	512.51	Joback Method
dvisc	0.0001488	Pa×s	575.78	Joback Method
dvisc	0.0000982	Pa×s	639.05	Joback Method
dvisc	0.0000698	Pa×s	702.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47974&Units=SI
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

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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