

Hexadecane, 7-butyl

Inchi: InChI=1S/C20H42/c1-4-7-10-12-13-14-16-19-20(17-9-6-3)18-15-11-8-5-2/h20H,4-19H2,1
InchiKey: SLPCWYHEQGSCLC-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCCCCCCC(CCCC)CCCCC
Mol. weight [g/mol]: 282.55

Physical Properties

Property code	Value	Unit	Source
gf	115.08	kJ/mol	Joback Method
hf	-461.41	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.904		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	656.56	K	Joback Method
tc	818.58	K	Joback Method
tf	300.16	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.82	J/molxK	656.56	Joback Method
cpg	862.00	J/molxK	683.56	Joback Method
cpg	882.29	J/molxK	710.57	Joback Method
cpg	901.73	J/molxK	737.57	Joback Method
cpg	920.35	J/molxK	764.58	Joback Method
cpg	938.17	J/molxK	791.58	Joback Method
cpg	955.21	J/molxK	818.58	Joback Method

dvisc	0.0051032	Paxs	300.16	Joback Method
dvisc	0.0014944	Paxs	359.56	Joback Method
dvisc	0.0006199	Paxs	418.96	Joback Method
dvisc	0.0003200	Paxs	478.36	Joback Method
dvisc	0.0001911	Paxs	537.76	Joback Method
dvisc	0.0001265	Paxs	597.16	Joback Method
dvisc	0.0000902	Paxs	656.56	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=R8630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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