

Hexadecane, 8-butyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H42/c1-4-7-10-12-14-16-19-20(17-9-6-3)18-15-13-11-8-5-2/h20H,4-19H2,1

NWSIMTXGGKCNLC-UHFFFAOYSA-N

C20H42

CCCCCCCCC(CCCC)CCCCCCC

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	1870.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1870.00		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/mol×K	656.56	Joback Method
cpg	862.00	J/mol×K	683.56	Joback Method
cpg	882.29	J/mol×K	710.57	Joback Method
cpg	901.73	J/mol×K	737.57	Joback Method
cpg	920.35	J/mol×K	764.58	Joback Method
cpg	938.17	J/mol×K	791.58	Joback Method
cpg	955.21	J/mol×K	818.58	Joback Method

dvisc	0.0051032	Pa×s	300.16	Joback Method
dvisc	0.0014944	Pa×s	359.56	Joback Method
dvisc	0.0006199	Pa×s	418.96	Joback Method
dvisc	0.0003200	Pa×s	478.36	Joback Method
dvisc	0.0001911	Pa×s	537.76	Joback Method
dvisc	0.0001265	Pa×s	597.16	Joback Method
dvisc	0.0000902	Pa×s	656.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R8774&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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