

6,6-Diethylhexadecane

Inchi:	InChI=1S/C20H42/c1-5-9-11-12-13-14-15-17-19-20(7-3,8-4)18-16-10-6-2/h5-19H2,1-4H3
InchiKey:	DBQGQSCHJJUMOP-UHFFFAOYSA-N
Formula:	C20H42
SMILES:	CCCCCCCCCCC(CC)(CC)CCCC
Mol. weight [g/mol]:	282.55

Physical Properties

Property code	Value	Unit	Source
gf	120.36	kJ/mol	Joback Method
hf	-464.88	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	58.82	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.904		Crippen Method
mvol	292.660	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	1894.00		NIST Webbook
tb	653.77	K	Joback Method
tc	818.91	K	Joback Method
tf	317.58	K	Joback Method
vc	1.145	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.36	J/molxK	653.77	Joback Method
cpg	863.80	J/molxK	681.29	Joback Method
cpg	884.29	J/molxK	708.82	Joback Method
cpg	903.87	J/molxK	736.34	Joback Method
cpg	922.58	J/molxK	763.87	Joback Method
cpg	940.45	J/molxK	791.39	Joback Method
cpg	957.52	J/molxK	818.91	Joback Method
dvisc	0.0043077	Paxs	317.58	Joback Method
dvisc	0.0013647	Paxs	373.61	Joback Method

dvisc	0.0005835	Paxs	429.64	Joback Method
dvisc	0.0003035	Paxs	485.67	Joback Method
dvisc	0.0001807	Paxs	541.71	Joback Method
dvisc	0.0001186	Paxs	597.74	Joback Method
dvisc	0.0000837	Paxs	653.77	Joback Method

Sources

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=U360414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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