

Dodecane, 6,7-dibutyl

Inchi:	InChI=1S/C20H42/c1-5-9-13-17-19(15-11-7-3)20(16-12-8-4)18-14-10-6-2/h19-20H,5-18H
InchiKey:	YCLOGUQQHLMMHU-UHFFFAOYSA-N
Formula:	C20H42
SMILES:	CCCCC(CCCC)C(CCCC)CCCC
Mol. weight [g/mol]:	282.55

Physical Properties

Property code	Value	Unit	Source
gf	112.64	kJ/mol	Joback Method
hf	-466.69	kJ/mol	Joback Method
hfus	40.51	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.760		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	656.12	K	Joback Method
tc	819.90	K	Joback Method
tf	285.16	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.15	J/molxK	656.12	Joback Method
cpg	862.59	J/molxK	683.42	Joback Method
cpg	883.13	J/molxK	710.71	Joback Method
cpg	902.79	J/molxK	738.01	Joback Method
cpg	921.59	J/molxK	765.31	Joback Method
cpg	939.58	J/molxK	792.60	Joback Method
cpg	956.77	J/molxK	819.90	Joback Method
dvisc	0.0075349	Paxs	285.16	Joback Method

dvisc	0.0018250	Paxs	346.99	Joback Method
dvisc	0.0006788	Paxs	408.81	Joback Method
dvisc	0.0003274	Paxs	470.64	Joback Method
dvisc	0.0001870	Paxs	532.47	Joback Method
dvisc	0.0001200	Paxs	594.29	Joback Method
dvisc	0.0000838	Paxs	656.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R8994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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