

6,6-Diethyloctadecane

Other names:	6,6-Diethyloctadecane
Inchi:	InChI=1S/C22H46/c1-5-9-11-12-13-14-15-16-17-19-21-22(7-3,8-4)20-18-10-6-2/h5-21H2
InchiKey:	GMZYILNPDQRDQY-UHFFFAOYSA-N
Formula:	C22H46
SMILES:	CCCCCCCCCCCC(CC)(CC)CCCC
Mol. weight [g/mol]:	310.60

Physical Properties

Property code	Value	Unit	Source
gf	137.20	kJ/mol	Joback Method
hf	-506.16	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	699.53	K	Joback Method
tc	866.63	K	Joback Method
tf	340.12	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.48	J/molxK	699.53	Joback Method
cpg	985.57	J/molxK	727.38	Joback Method
cpg	1006.67	J/molxK	755.23	Joback Method
cpg	1026.82	J/molxK	783.08	Joback Method
cpg	1046.05	J/molxK	810.93	Joback Method
cpg	1064.42	J/molxK	838.78	Joback Method
cpg	1081.96	J/molxK	866.63	Joback Method

dvisc	0.0033295	Paxs	340.12	Joback Method
dvisc	0.0010494	Paxs	400.02	Joback Method
dvisc	0.0004468	Paxs	459.92	Joback Method
dvisc	0.0002316	Paxs	519.83	Joback Method
dvisc	0.0001375	Paxs	579.73	Joback Method
dvisc	0.0000900	Paxs	639.63	Joback Method
dvisc	0.0000634	Paxs	699.53	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=U360418&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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