1-Nonadecyne

Inchi: InChI=1S/C19H36/c1-3-5-7-9-11-13-15-17-19-18-16-14-12-10-8-6-4-2/h1H,4-19H2,2H3
InchiKey: KOGJOFWBMIOBCC-UHFFFAOYSA-N
Formula: C19H36
SMILES: C#CCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 264.49
CAS: 26186-01-6

Physical Properties

Property code	Value	Unit	Source
af	0.7350		KDB
gf	332.17	kJ/mol	Joback Method
hf	-143.59	kJ/mol	Joback Method
hfus	47.94	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.881		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1190.00	kPa	KDB
tb	600.20	K	KDB
tc	758.90	K	KDB
tf	306.00	K	KDB
vc	1.062	m3/kmol	KDB
zc	0.2001920		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.76	J/mol×K	624.24	Joback Method
cpg	754.48	J/mol×K	651.76	Joback Method
cpg	773.37	J/mol×K	679.29	Joback Method
cpg	791.46	J/mol×K	706.81	Joback Method
cpg	808.77	J/mol×K	734.34	Joback Method
cpg	825.33	J/mol×K	761.86	Joback Method
cpg	841.18	J/mol×K	789.39	Joback Method

hvapt	66.90	kJ/mol	549.50	NIST Webbook

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol444.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26186016&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

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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