

2-Methyl-7-octadecyne

Other names:	2-Methyl-7-octadecyne
Inchi:	InChI=1S/C19H36/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)3/h19H,4-12,15-18H
InchiKey:	WQMKDHFREUPHQQE-UHFFFAOYSA-N
Formula:	C19H36
SMILES:	CCCCCCCCCCC#CCCCC(C)C
Mol. weight [g/mol]:	264.50

Physical Properties

Property code	Value	Unit	Source
af	0.6987		Cheméo Relay (1.0)
gf	309.46	kJ/mol	Joback Method
hf	-194.65	kJ/mol	Cheméo Relay (1.0)
hfus	44.57	kJ/mol	Joback Method
hvap	83.74	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-7.62		Cheméo Relay (1.0)
logp	6.737		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
tb	560.31	K	Cheméo Relay (1.0)
tc	749.53	K	Cheméo Relay (1.0)
tf	265.15	K	Cheméo Relay (1.0)
vc	1.030	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.51	J/mol×K	642.68	Joback Method
cpg	763.02	J/mol×K	671.76	Joback Method
cpg	782.62	J/mol×K	700.83	Joback Method
cpg	801.36	J/mol×K	729.91	Joback Method
cpg	819.26	J/mol×K	758.99	Joback Method
cpg	836.34	J/mol×K	788.07	Joback Method
cpg	852.64	J/mol×K	817.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35354382&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
ie:	Ionization energy
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

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