7-Octadecyne, 2-methyl-

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: WQMKDHREUPHQQE-UHFFFAOYSA-N
Formula: C19H36
SMILES: CCCCCCCCCCC#CCCCCC(C)C
Mol. weight [g/mol]: 264.49
CAS: 35354-38-2

Physical Properties

Property code	Value	Unit	Source
gf	309.46	kJ/mol	Joback Method
hf	-168.47	kJ/mol	Joback Method
hfus	44.57	kJ/mol	Joback Method
hvap	59.65	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.737		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
tb	642.68	K	Joback Method
tc	817.14	K	Joback Method
tf	394.99	K	Joback Method
vc	1.056	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C35354382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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