3-Octadecyne

Inchi: InChI=1S/C18H34/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3-5,7,9-18H2,1-2H3
InchiKey: UQMLWEGZEBCVLH-UHFFFAOYSA-N
Formula: C18H34
SMILES: CCC#CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 250.46
CAS: 61886-64-4

Physical Properties

Property code	Value	Unit	Source
gf	303.48	kJ/mol	Joback Method
hf	-142.55	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	57.81	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.491		Crippen Method
mcvol	255.880	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
tb	620.24	K	Joback Method
tc	792.82	K	Joback Method
tf	398.72	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.31	J/mol×K	764.06	Joback Method
cpg	685.49	J/mol×K	620.24	Joback Method
cpg	705.29	J/mol×K	649.00	Joback Method
cpg	724.24	J/mol×K	677.77	Joback Method
cpg	742.38	J/mol×K	706.53	Joback Method
cpg	759.73	J/mol×K	735.29	Joback Method
cpg	792.16	J/mol×K	792.82	Joback Method
hvapt	64.50	kJ/mol	535.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55327e+01
Coeff. B	-5.26477e+03
Coeff. C	-1.04378e+02
Temperature range (K), min.	449.72
Temperature range (K), max.	619.46

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=C61886644&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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