2-methyl-1-heptadecene

Inchi: InChI=1S/C18H36/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2)3/h2,4-17H2,1,3H3
InchiKey: ZKRHEOXJNQPNQD-UHFFFAOYSA-N
Formula: C18H36
SMILES: C=C(C)CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 252.48
CAS: 42764-74-9

Physical Properties

Property code	Value	Unit	Source
gf	179.97	kJ/mol	Joback Method
hf	-299.21	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	55.07	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	7.044		Crippen Method
mcvol	260.180	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	1787.00		NIST Webbook
tb	607.80	K	Joback Method
tc	770.33	K	Joback Method
tf	276.90	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.94	J/mol×K	607.80	Joback Method
cpg	720.78	J/mol×K	634.89	Joback Method
cpg	739.80	J/mol×K	661.98	Joback Method
cpg	758.04	J/mol×K	689.06	Joback Method
cpg	775.51	J/mol×K	716.15	Joback Method
cpg	792.24	J/mol×K	743.24	Joback Method
cpg	808.26	J/mol×K	770.33	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55122e+01
Coeff. B	-5.28146e+03
Coeff. C	-9.40000e+01
Temperature range (K), min.	440.90
Temperature range (K), max.	611.76

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=R205800&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor 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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