5-Methylheptadecane

Inchi: InChI=1S/C18H38/c1-4-6-8-9-10-11-12-13-14-15-17-18(3)16-7-5-2/h18H,4-17H2,1-3H3
InchiKey: WHUUMUMJALVXPL-UHFFFAOYSA-N
Formula: C18H38
SMILES: CCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 254.49
CAS: 26730-95-0

Physical Properties

Property code	Value	Unit	Source
af	0.7463		Cheméo Relay (1.0)
gf	98.24	kJ/mol	Joback Method
hf	-424.37	kJ/mol	Cheméo Relay (1.0)
hfus	38.85	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-8.02		Cheméo Relay (1.0)
logp	7.124		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
tb	560.85	K	Cheméo Relay (1.0)
tc	726.02	K	Cheméo Relay (1.0)
tf	258.07	K	Cheméo Relay (1.0)
vc	1.038	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.70	J/mol×K	744.91	Joback Method
cpg	834.20	J/mol×K	771.74	Joback Method
cpg	744.17	J/mol×K	637.62	Joback Method
cpg	763.72	J/mol×K	664.45	Joback Method
cpg	782.48	J/mol×K	691.27	Joback Method
cpg	800.46	J/mol×K	718.09	Joback Method
cpg	723.79	J/mol×K	610.80	Joback Method

dvisc	0.0007754	Pa×s	388.68	Joback Method
dvisc	0.0018624	Pa×s	333.15	Joback Method
dvisc	0.0063506	Pa×s	277.62	Joback Method
dvisc	0.0004019	Pa×s	444.21	Joback Method
dvisc	0.0002411	Pa×s	499.74	Joback Method
dvisc	0.0001602	Pa×s	555.27	Joback Method
dvisc	0.0001146	Pa×s	610.80	Joback Method
hvapt	61.10	kJ/mol	506.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73381e+01
Coeff. B	-7.41374e+03
Coeff. C	1.96100e+00
Temperature range (K), min.	432.85
Temperature range (K), max.	614.48

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26730950&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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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