DECANOIC ACID, 2-HEXYL-

Other names:	2-Hexyldecansaeure
	2-hexyldecanoic acid
	2-n-Hexyldecanoic acid
	7-Pentadecanecarboxylic acid
Inchi:	InChI=1S/C16H32O2/c1-3-5-7-9-10-12-14-15(16(17)18)13-11-8-6-4-2/h15H,3-14H2,1-2H
InchiKey:	JMOLZNNXZPAGBH-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCC(CCCCCC)C(=O)O
Mol. weight [g/mol]:	256.43
CAS:	25354-97-6

Physical Properties

Property code	Value	Unit	Source
af	0.9596		Cheméo Relay (1.0)
gf	-184.34	kJ/mol	Joback Method
hf	-727.15	kJ/mol	Cheméo Relay (1.0)
hfus	39.36	kJ/mol	Joback Method
hvap	100.78	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-5.46		Cheméo Relay (1.0)
logp	5.408		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
tb	576.65	K	Cheméo Relay (1.0)
tc	777.56	K	Cheméo Relay (1.0)
tf	289.65	K	Cheméo Relay (1.0)
vc	0.909	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.27	J/mol×K	711.09	Joback Method
cpg	736.41	J/mol×K	739.43	Joback Method
cpg	751.80	J/mol×K	767.78	Joback Method

cpg	766.47	J/mol×K	796.12	Joback Method
cpg	780.45	J/mol×K	824.46	Joback Method
cpg	793.76	J/mol×K	852.80	Joback Method
cpg	806.41	J/mol×K	881.15	Joback Method
dvisc	0.0052083	Pa×s	365.83	Joback Method
dvisc	0.0012596	Pa×s	423.37	Joback Method
dvisc	0.0004279	Pa×s	480.92	Joback Method
dvisc	0.0001831	Pa×s	538.46	Joback Method
dvisc	0.0000923	Pa×s	596.00	Joback Method
dvisc	0.0000525	Pa×s	653.55	Joback Method
dvisc	0.0000327	Pa×s	711.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59625e+01
Coeff. B	-5.73094e+03
Coeff. C	-1.14108e+02
Temperature range (K), min.	479.72
Temperature range (K), max.	652.17

Sources

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=C25354976&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):

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
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