

2-Hexyldecanoic acid

Other names:	2-Hexyldecansaeure 2-n-Hexyldecanoic acid 7-Pentadecanecarboxylic acid Decanoic acid, 2-hexyl-
Inchi:	InChI=1S/C16H32O2/c1-3-5-7-9-10-12-14-15(16(17)18)13-11-8-6-4-2/h15H,3-14H2,1-2H1
InchiKey:	JMOLZNNXZPAGBH-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCC(CCCCC)C(=O)O
Mol. weight [g/mol]:	256.42
CAS:	25354-97-6

Physical Properties

Property code	Value	Unit	Source
gf	-184.34	kJ/mol	Joback Method
hf	-643.66	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.408		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
tb	711.09	K	Joback Method
tc	881.15	K	Joback Method
tf	365.83	K	Joback Method
vc	0.951	m3/kmol	Joback Method

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	$\ln(P_{vp}) = A + B/(T + C)$
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

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=C25354976&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
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
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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