2-octyldecanoic acid

Inchi: InChI=1S/C18H36O2/c1-3-5-7-9-11-13-15-17(18(19)20)16-14-12-10-8-6-4-2/h17H,3-16H
InchiKey: OYYXZGFIZTYYRB-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCC(CCCCCCCC)C(=O)O
Mol. weight [g/mol]: 284.48
CAS: 619-39-6

Physical Properties

Property code	Value	Unit	Source
af	1.0299		Cheméo Relay (1.0)
gf	-167.50	kJ/mol	Joback Method
hf	-767.79	kJ/mol	Cheméo Relay (1.0)
hfus	44.54	kJ/mol	Joback Method
hvap	107.86	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-6.14		Cheméo Relay (1.0)
logp	6.188		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
tb	591.11	K	Cheméo Relay (1.0)
tc	792.06	K	Cheméo Relay (1.0)
tf	307.41	K	Cheméo Relay (1.0)
vc	1.020	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.93	J/mol×K	756.85	Joback Method
cpg	853.09	J/mol×K	785.85	Joback Method
cpg	869.43	J/mol×K	814.86	Joback Method
cpg	884.97	J/mol×K	843.86	Joback Method
cpg	899.74	J/mol×K	872.86	Joback Method
cpg	913.77	J/mol×K	901.86	Joback Method
cpg	927.10	J/mol×K	930.87	Joback Method

dvisc	0.0034379	Pa×s	388.37	Joback Method
dvisc	0.0008398	Pa×s	449.78	Joback Method
dvisc	0.0002878	Pa×s	511.20	Joback Method
dvisc	0.0001241	Pa×s	572.61	Joback Method
dvisc	0.0000630	Pa×s	634.02	Joback Method
dvisc	0.0000360	Pa×s	695.44	Joback Method
dvisc	0.0000226	Pa×s	756.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67152e+01
Coeff. B	-6.28483e+03
Coeff. C	-1.23143e+02
Temperature range (K), min.	505.72
Temperature range (K), max.	674.26

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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):
Cheméo Relay (1.0, beta):

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

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