2-Methyldodecanoic acid

Inchi: InChI=1S/C13H26O2/c1-3-4-5-6-7-8-9-10-11-12(2)13(14)15/h12H,3-11H2,1-2H3,(H,14,1
InchiKey: ONEKODVPFBOORO-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCCCCC(C)C(=O)O
Mol. weight [g/mol]: 214.35
CAS: 2874-74-0

Physical Properties

Property code	Value	Unit	Source
af	0.8738		Cheméo Relay (1.0)
gf	-209.60	kJ/mol	Joback Method
hf	-674.66	kJ/mol	Cheméo Relay (1.0)
hfus	31.59	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-4.39		Cheméo Relay (1.0)
logp	4.238		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
tb	544.16	K	Cheméo Relay (1.0)
tc	742.16	K	Cheméo Relay (1.0)
tf	288.80	K	Cheméo Relay (1.0)
vc	0.757	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.48	J/mol×K	642.45	Joback Method
cpg	570.05	J/mol×K	670.47	Joback Method
cpg	583.97	J/mol×K	698.50	Joback Method
cpg	597.27	J/mol×K	726.52	Joback Method
cpg	609.97	J/mol×K	754.55	Joback Method
cpg	622.08	J/mol×K	782.57	Joback Method
cpg	633.62	J/mol×K	810.60	Joback Method

dvisc	0.0097836	Pa×s	332.02	Joback Method
dvisc	0.0023257	Pa×s	383.76	Joback Method
dvisc	0.0007778	Pa×s	435.50	Joback Method
dvisc	0.0003282	Pa×s	487.23	Joback Method
dvisc	0.0001635	Pa×s	538.97	Joback Method
dvisc	0.0000920	Pa×s	590.71	Joback Method
dvisc	0.0000568	Pa×s	642.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56459e+01
Coeff. B	-5.27447e+03
Coeff. C	-1.02293e+02
Temperature range (K), min.	445.72
Temperature range (K), max.	612.67

Sources

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):

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=C2874740&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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