11-Dodecenoic acid

Inchi: InChI=1S/C12H22O2/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2H,1,3-11H2,(H,13,14)
InchiKey: GZZPOFFXKUVNSW-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=CCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 198.30
CAS: 65423-25-8

Physical Properties

Property code	Value	Unit	Source
gf	-127.74	kJ/mol	Joback Method
hf	-430.39	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	65.06	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.768		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
ripol	2565.00		NIST Webbook
ripol	2565.00		NIST Webbook
tb	616.69	K	Joback Method
tc	784.80	K	Joback Method
tf	333.99	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.13	J/mol×K	616.69	Joback Method
cpg	494.34	J/mol×K	644.71	Joback Method
cpg	506.96	J/mol×K	672.73	Joback Method
cpg	519.02	J/mol×K	700.74	Joback Method
cpg	530.52	J/mol×K	728.76	Joback Method
cpg	541.50	J/mol×K	756.78	Joback Method
cpg	551.98	J/mol×K	784.80	Joback Method

dvisc	0.0075368	Pa×s	333.99	Joback Method
dvisc	0.0021882	Pa×s	381.11	Joback Method
dvisc	0.0008340	Pa×s	428.22	Joback Method
dvisc	0.0003849	Pa×s	475.34	Joback Method
dvisc	0.0002042	Pa×s	522.46	Joback Method
dvisc	0.0001203	Pa×s	569.57	Joback Method
dvisc	0.0000769	Pa×s	616.69	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39339e+01
Coeff. B	-4.61171e+03
Coeff. C	-9.93740e+01
Temperature range (K), min.	437.32
Temperature range (K), max.	634.23

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=C65423258&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume