2-Dodecenoic acid

Other names: Dodec-2-enoic acid
Inchi: InChI=1S/C12H22O2/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h10-11H,2-9H2,1H3,(H,13,14)/b
InchiKey: PAWGRNGPMLVJQH-ZHACJKMWSA-N
Formula: C12H22O2
SMILES: CCCCCCCCCC=CC(=O)O
Mol. weight [g/mol]: 198.30
CAS: 4412-16-2

Physical Properties

Property code	Value	Unit	Source
gf	-135.36	kJ/mol	Joback Method
hf	-438.60	kJ/mol	Joback Method
hfus	32.73	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.768		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
tb	624.17	K	Joback Method
tc	795.47	K	Joback Method
tf	330.67	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.07	J/mol×K	624.17	Joback Method
cpg	495.33	J/mol×K	652.72	Joback Method
cpg	507.99	J/mol×K	681.27	Joback Method
cpg	520.06	J/mol×K	709.82	Joback Method
cpg	531.58	J/mol×K	738.37	Joback Method
cpg	542.56	J/mol×K	766.92	Joback Method
cpg	553.04	J/mol×K	795.47	Joback Method
dvisc	0.0075567	Pa×s	330.67	Joback Method

dvisc	0.0020223	Pa×s	379.59	Joback Method
dvisc	0.0007313	Pa×s	428.50	Joback Method
dvisc	0.0003257	Pa×s	477.42	Joback Method
dvisc	0.0001686	Pa×s	526.34	Joback Method
dvisc	0.0000976	Pa×s	575.25	Joback Method
dvisc	0.0000616	Pa×s	624.17	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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C4412162&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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