Formic acid, decyl ester

Other names: Decyl formate
n-Decyl methanoate
Inchi: InChI=1S/C11H22O2/c1-2-3-4-5-6-7-8-9-10-13-11-12/h11H,2-10H2,1H3
InchiKey: BCLJZFLDSCTULJ-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCCCCCCCCCOC=O
Mol. weight [g/mol]: 186.29
CAS: 5451-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-162.78	kJ/mol	Joback Method
hf	-488.17	kJ/mol	Joback Method
hfus	27.72	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1342.00		NIST Webbook
tb	522.16	K	Joback Method
tc	689.35	K	Joback Method
tf	277.96	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.57	J/mol×K	522.16	Joback Method
cpg	430.19	J/mol×K	550.03	Joback Method
cpg	444.27	J/mol×K	577.89	Joback Method

cpg	457.80	J/mol×K	605.76	Joback Method
cpg	470.80	J/mol×K	633.62	Joback Method
cpg	483.28	J/mol×K	661.49	Joback Method
cpg	495.24	J/mol×K	689.35	Joback Method
dvisc	0.0036674	Pa×s	277.96	Joback Method
dvisc	0.0017096	Pa×s	318.66	Joback Method
dvisc	0.0009474	Pa×s	359.36	Joback Method
dvisc	0.0005920	Pa×s	400.06	Joback Method
dvisc	0.0004035	Pa×s	440.76	Joback Method
dvisc	0.0002934	Pa×s	481.46	Joback Method
dvisc	0.0002242	Pa×s	522.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.78331e+01
Coeff. B	-5.40892e+03
Coeff. C	-8.46400e+01
Temperature range (K), min.	392.92
Temperature range (K), max.	516.61

Sources

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
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=C5451525&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume