Decanoic acid, 2-methyl-

Other names: 2-Methyldecanoic acid
Inchi: InChI=1S/C11H22O2/c1-3-4-5-6-7-8-9-10(2)11(12)13/h10H,3-9H2,1-2H3,(H,12,13)
InchiKey: SAOSCTYRONNFTC-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCCCCCCCC(C)C(=O)O
Mol. weight [g/mol]: 186.29
CAS: 24323-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-226.44	kJ/mol	Joback Method
hf	-540.46	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.458		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	596.69	K	Joback Method
tc	765.61	K	Joback Method
tf	309.48	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.39	J/mol×K	596.69	Joback Method
cpg	465.76	J/mol×K	624.84	Joback Method
cpg	478.55	J/mol×K	653.00	Joback Method
cpg	490.78	J/mol×K	681.15	Joback Method
cpg	502.47	J/mol×K	709.30	Joback Method
cpg	513.62	J/mol×K	737.46	Joback Method
cpg	524.26	J/mol×K	765.61	Joback Method
dvisc	0.0149700	Pa×s	309.48	Joback Method

dvisc	0.0035118	Pa×s	357.35	Joback Method
dvisc	0.0011604	Pa×s	405.22	Joback Method
dvisc	0.0004845	Pa×s	453.09	Joback Method
dvisc	0.0002391	Pa×s	500.95	Joback Method
dvisc	0.0001334	Pa×s	548.82	Joback Method
dvisc	0.0000818	Pa×s	596.69	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54533e+01
Coeff. B	-4.96291e+03
Coeff. C	-9.36750e+01
Temperature range (K), min.	420.92
Temperature range (K), max.	583.02

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24323237&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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