Isoundecanoic acid

Other names: 10-methylundecanoic acid
Inchi: InChI=1S/C12H24O2/c1-11(2)9-7-5-3-4-6-8-10-12(13)14/h11H,3-10H2,1-2H3,(H,13,14)
InchiKey: QJRRBVNPIKYRQJ-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CC(C)CCCCCCCCC(=O)O
Mol. weight [g/mol]: 200.32
CAS: 2724-56-3

Physical Properties

Property code	Value	Unit	Source
gf	-218.02	kJ/mol	Joback Method
hf	-561.10	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.848		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1399.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	619.57	K	Joback Method
tc	787.94	K	Joback Method
tf	315.70 ± 1.00	K	NIST Webbook
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.20	J/mol×K	619.57	Joback Method
cpg	517.19	J/mol×K	647.63	Joback Method
cpg	530.57	J/mol×K	675.69	Joback Method
cpg	543.36	J/mol×K	703.75	Joback Method
cpg	555.57	J/mol×K	731.81	Joback Method
cpg	567.23	J/mol×K	759.87	Joback Method

cpg	578.34	J/mol×K	787.94	Joback Method
dvisc	0.0120962	Pa×s	320.75	Joback Method
dvisc	0.0028570	Pa×s	370.55	Joback Method
dvisc	0.0009499	Pa×s	420.36	Joback Method
dvisc	0.0003988	Pa×s	470.16	Joback Method
dvisc	0.0001977	Pa×s	519.96	Joback Method
dvisc	0.0001108	Pa×s	569.77	Joback Method
dvisc	0.0000682	Pa×s	619.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55220e+01
Coeff. B	-5.10866e+03
Coeff. C	-9.79840e+01
Temperature range (K), min.	433.32
Temperature range (K), max.	598.31

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=C2724563&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume