Dec-4-enal

Other names: 4-Decenal
Inchi: InChI=1S/C10H18O/c1-2-3-4-5-6-7-8-9-10-11/h6-7,10H,2-5,8-9H2,1H3
InchiKey: CWRKZMLUDFBPAO-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CCCCCC=CCCC=O
Mol. weight [g/mol]: 154.25
CAS: 30390-50-2

Physical Properties

Property code	Value	Unit	Source
gf	14.02	kJ/mol	Joback Method
hf	-218.09	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1172.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1194.00		NIST Webbook
tb	481.02	K	Joback Method
tc	657.18	K	Joback Method
tf	239.38	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.08	J/mol×K	481.02	Joback Method
cpg	339.86	J/mol×K	510.38	Joback Method
cpg	353.02	J/mol×K	539.74	Joback Method
cpg	365.57	J/mol×K	569.10	Joback Method

cpg	377.54	J/mol×K	598.46	Joback Method
cpg	388.96	J/mol×K	627.82	Joback Method
cpg	399.85	J/mol×K	657.18	Joback Method
dvisc	0.0048073	Pa×s	239.38	Joback Method
dvisc	0.0020448	Pa×s	279.65	Joback Method
dvisc	0.0010787	Pa×s	319.93	Joback Method
dvisc	0.0006565	Pa×s	360.20	Joback Method
dvisc	0.0004415	Pa×s	400.47	Joback Method
dvisc	0.0003193	Pa×s	440.75	Joback Method
dvisc	0.0002437	Pa×s	481.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44415e+01
Coeff. B	-4.15084e+03
Coeff. C	-7.82400e+01
Temperature range (K), min.	371.50
Temperature range (K), max.	532.87

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30390502&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume