

2-tridecenal

Other names:	Tridec-2-enal
Inchi:	InChI=1S/C13H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h11-13H,2-10H2,1H3
InchiKey:	VMUNAKQXJLHODT-UHFFFAOYSA-N
Formula:	C13H24O
SMILES:	CCCCCCCCCCC=CC=O
Mol. weight [g/mol]:	196.33
CAS:	7774-82-5

Physical Properties

Property code	Value	Unit	Source
gf	39.28	kJ/mol	Joback Method
hf	-280.01	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.272		Crippen Method
mcvol	191.300	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1868.00		NIST Webbook
tb	549.66	K	Joback Method
tc	721.56	K	Joback Method
tf	273.19	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.87	J/mol×K	549.66	Joback Method

cpg	540.69	J/mol×K	692.91	Joback Method
cpg	527.44	J/mol×K	664.26	Joback Method
cpg	513.56	J/mol×K	635.61	Joback Method
cpg	499.02	J/mol×K	606.96	Joback Method
cpg	483.80	J/mol×K	578.31	Joback Method
cpg	553.33	J/mol×K	721.56	Joback Method
dvisc	0.0001974	Pa×s	549.66	Joback Method
dvisc	0.0002621	Pa×s	503.58	Joback Method
dvisc	0.0003685	Pa×s	457.50	Joback Method
dvisc	0.0005592	Pa×s	411.43	Joback Method
dvisc	0.0009427	Pa×s	365.35	Joback Method
dvisc	0.0018476	Pa×s	319.27	Joback Method
dvisc	0.0045438	Pa×s	273.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42344e+01
Coeff. B	-4.46152e+03
Coeff. C	-9.24240e+01
Temperature range (K), min.	412.32
Temperature range (K), max.	592.43

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=C7774825&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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