

11-methyldodecanoic acid

Other names:	isotridecanoic acid
Inchi:	InChI=1S/C13H26O2/c1-12(2)10-8-6-4-3-5-7-9-11-13(14)15/h12H,3-11H2,1-2H3,(H,14,1
InchiKey:	SIOLDWZBFABPJU-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CC(C)CCCCCCCCC(=O)O
Mol. weight [g/mol]:	214.34
CAS:	25448-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-209.60	kJ/mol	Joback Method
hf	-581.74	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.238		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
ripol	2555.00		NIST Webbook
tb	642.45	K	Joback Method
tc	810.60	K	Joback Method
tf	332.02	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.48	J/molxK	642.45	Joback Method
cpg	570.05	J/molxK	670.47	Joback Method
cpg	583.97	J/molxK	698.50	Joback Method
cpg	597.27	J/molxK	726.52	Joback Method
cpg	609.97	J/molxK	754.55	Joback Method
cpg	622.08	J/molxK	782.57	Joback Method
cpg	633.62	J/molxK	810.60	Joback Method

dvisc	0.0097836	Paxs	332.02	Joback Method
dvisc	0.0023257	Paxs	383.76	Joback Method
dvisc	0.0007778	Paxs	435.50	Joback Method
dvisc	0.0003282	Paxs	487.24	Joback Method
dvisc	0.0001635	Paxs	538.97	Joback Method
dvisc	0.0000920	Paxs	590.71	Joback Method
dvisc	0.0000568	Paxs	642.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56459e+01
Coeff. B	-5.27447e+03
Coeff. C	-1.02293e+02
Temperature range (K), min.	445.72
Temperature range (K), max.	612.67

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25448242&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/83-242-1/11-methyldodecanoic-acid.pdf>

Generated by Cheméo on 2025-02-18 15:39:43.489278553 +0000 UTC m=+3101399.336204182.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.