

Dodecyl formate

Other names:	dodecyl methanoate
Inchi:	InChI=1S/C13H26O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-13-14/h13H,2-12H2,1H3
InchiKey:	WPSGFSPBRBRLIQ-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	214.34
CAS:	28303-42-6

Physical Properties

Property code	Value	Unit	Source
gf	-145.94	kJ/mol	Joback Method
hf	-529.45	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	567.92	K	Joback Method
tc	733.32	K	Joback Method
tf	300.50	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.65	J/molxK	567.92	Joback Method
cpg	588.49	J/molxK	705.75	Joback Method
cpg	574.93	J/molxK	678.19	Joback Method
cpg	560.77	J/molxK	650.62	Joback Method

cpg	546.02	J/molxK	623.05	Joback Method
cpg	530.65	J/molxK	595.49	Joback Method
cpg	601.48	J/molxK	733.32	Joback Method
dvisc	0.0001868	Paxs	567.92	Joback Method
dvisc	0.0002466	Paxs	523.35	Joback Method
dvisc	0.0003426	Paxs	478.78	Joback Method
dvisc	0.0005093	Paxs	434.21	Joback Method
dvisc	0.0008289	Paxs	389.64	Joback Method
dvisc	0.0015302	Paxs	345.07	Joback Method
dvisc	0.0033880	Paxs	300.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.90325e+01
Coeff. B	-6.20920e+03
Coeff. C	-9.68720e+01
Temperature range (K), min.	428.12
Temperature range (K), max.	549.41

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C28303426&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
h vap:	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
r in pol:	Non-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/83-244-9/Dodecyl-formate.pdf>

Generated by Cheméo on 2024-04-23 12:40:15.59521677 +0000 UTC m=+16165264.515794086.

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