

(2E,6Z)-dodeca-2,6-dienal

Inchi:	InChI=1S/C12H20O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h6-7,10-12H,2-5,8-9H2,1H3/b7-6-,1
InchiKey:	VPEGROOEBNSCCL-JFEAUALZSA-N
Formula:	C12H20O
SMILES:	CCCCC=CCCC=CC=O
Mol. weight [g/mol]:	180.29
CAS:	21662-13-5

Physical Properties

Property code	Value	Unit	Source
gf	111.08	kJ/mol	Joback Method
hf	-142.15	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.658		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1448.70		NIST Webbook
tb	530.94	K	Joback Method
tc	711.41	K	Joback Method
tf	256.84	K	Joback Method
vc	0.684	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.00	J/molxK	530.94	Joback Method
cpg	415.94	J/molxK	561.02	Joback Method
cpg	430.14	J/molxK	591.10	Joback Method
cpg	443.62	J/molxK	621.18	Joback Method
cpg	456.44	J/molxK	651.26	Joback Method
cpg	468.62	J/molxK	681.34	Joback Method
cpg	480.20	J/molxK	711.41	Joback Method
dvisc	0.0043899	Paxs	256.84	Joback Method

dvisc	0.0017283	Paxs	302.52	Joback Method
dvisc	0.0008690	Paxs	348.21	Joback Method
dvisc	0.0005125	Paxs	393.89	Joback Method
dvisc	0.0003373	Paxs	439.57	Joback Method
dvisc	0.0002402	Paxs	485.26	Joback Method
dvisc	0.0001813	Paxs	530.94	Joback Method

Sources

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=C21662135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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