

(E)-9,11-Dodecadienal

Inchi:	InChI=1S/C12H20O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-4,12H,1,5-11H2/b4-3+
InchiKey:	QQGSJQOOBIWRBK-ONEGZZNKSA-N
Formula:	C12H20O
SMILES:	C=CC=CCCCCCCCC=O
Mol. weight [g/mol]:	180.29
CAS:	97475-11-1

Physical Properties

Property code	Value	Unit	Source
gf	118.70	kJ/mol	Joback Method
hf	-133.94	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	48.31	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.658		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
tb	523.46	K	Joback Method
tc	699.81	K	Joback Method
tf	260.16	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.79	J/mol×K	523.46	Joback Method
cpg	466.96	J/mol×K	670.42	Joback Method
cpg	454.81	J/mol×K	641.03	Joback Method
cpg	442.05	J/mol×K	611.63	Joback Method
cpg	428.65	J/mol×K	582.24	Joback Method
cpg	414.57	J/mol×K	552.85	Joback Method
cpg	478.53	J/mol×K	699.81	Joback Method

dvisc	0.0002185	Paxs	523.46	Joback Method
dvisc	0.0002862	Paxs	479.58	Joback Method
dvisc	0.0003958	Paxs	435.69	Joback Method
dvisc	0.0005887	Paxs	391.81	Joback Method
dvisc	0.0009678	Paxs	347.93	Joback Method
dvisc	0.0018364	Paxs	304.04	Joback Method
dvisc	0.0043250	Paxs	260.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97475111&Units=SI
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
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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