

E5,Z7-dodecadienal

Inchi:	InChI=1S/C12H20O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h5-8,12H,2-4,9-11H2,1H3/b6-5-,8-7
InchiKey:	LDQDYNHCLZNOFB-IGTJQSIKSA-N
Formula:	C12H20O
SMILES:	CCCCC=CC=CCCC=O
Mol. weight [g/mol]:	180.29

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
ripol	1442.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1895.00		NIST Webbook
tb	530.94	K	Joback Method
tc	711.41	K	Joback Method
tf	256.84	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.00	J/molxK	530.94	Joback Method
cpg	468.62	J/molxK	681.34	Joback Method

cpg	456.44	J/molxK	651.26	Joback Method
cpg	443.62	J/molxK	621.18	Joback Method
cpg	430.14	J/molxK	591.10	Joback Method
cpg	415.94	J/molxK	561.02	Joback Method
cpg	480.20	J/molxK	711.41	Joback Method
dvisc	0.0001813	Paxs	530.94	Joback Method
dvisc	0.0002402	Paxs	485.26	Joback Method
dvisc	0.0003373	Paxs	439.57	Joback Method
dvisc	0.0005125	Paxs	393.89	Joback Method
dvisc	0.0008690	Paxs	348.21	Joback Method
dvisc	0.0017283	Paxs	302.52	Joback Method
dvisc	0.0043899	Paxs	256.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R517178&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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