6-dodecenal, E

Other names:	(E)-6-Dodecenal
Inchi:	InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h6-7,12H,2-5,8-11H2,1H3/b7-6+
InchiKey:	RKSXBPZEKYUCII-VOTSOKGWSA-N
Formula:	C12H22O
SMILES:	CCCCCC=CCCCCC=O
Mol. weight [g/mol]:	182.30

Physical Properties

Property code	Value	Unit	Source
gf	30.86	kJ/mol	Joback Method
hf	-259.37	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1396.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1731.00		NIST Webbook
tb	526.78	K	Joback Method
tc	700.00	K	Joback Method
tf	261.92	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.84	J/mol×K	526.78	Joback Method
cpg	434.14	J/mol×K	555.65	Joback Method
cpg	448.75	J/mol×K	584.52	Joback Method
cpg	462.70	J/mol×K	613.39	Joback Method
cpg	476.02	J/mol×K	642.26	Joback Method
cpg	488.73	J/mol×K	671.13	Joback Method

cpg	500.86	J/mol×K	700.00	Joback Method
dvisc	0.0046993	Pa×s	261.92	Joback Method
dvisc	0.0019373	Pa×s	306.06	Joback Method
dvisc	0.0009985	Pa×s	350.21	Joback Method
dvisc	0.0005970	Pa×s	394.35	Joback Method
dvisc	0.0003959	Pa×s	438.49	Joback Method
dvisc	0.0002830	Pa×s	482.64	Joback Method
dvisc	0.0002140	Pa×s	526.78	Joback Method

Sources

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=R265362&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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