TRANS-DODEC-5-ENAL

Other names: (E)-5-Dodecenal
5-Dodecenal, E
Inchi: InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h7-8,12H,2-6,9-11H2,1H3/b8-7+
InchiKey: MXYKXSMSECVABY-BQYQJAHWSA-N
Formula: C12H22O
SMILES: CCCCCC/C=C/CCCC=O
Mol. weight [g/mol]: 182.31

Physical Properties

Property code	Value	Unit	Source
af	0.5673		Cheméo Relay (1.0)
gf	30.86	kJ/mol	Joback Method
hf	-301.89	kJ/mol	Cheméo Relay (1.0)
hfus	29.33	kJ/mol	Joback Method
hvap	69.60	kJ/mol	NIST Webbook
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-4.29		Cheméo Relay (1.0)
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1394.00		NIST Webbook
ripol	1725.00		NIST Webbook
tb	511.90	K	Cheméo Relay (1.0)
tc	707.15	K	Cheméo Relay (1.0)
tf	262.13	K	Cheméo Relay (1.0)
vc	0.652	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68820348&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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