

(E)-11-(E)-13-Hexadecadienal

Inchi:	InChI=1S/C16H28O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h3-6,16H,2,7-15H2,1H
InchiKey:	ZTJGMVSDMQAJPE-VNKDHWASSA-N
Formula:	C16H28O
SMILES:	CCC=CC=CCCCCCCCCCC=O
Mol. weight [g/mol]:	236.39

Physical Properties

Property code	Value	Unit	Source
gf	144.76	kJ/mol	Joback Method
hf	-224.71	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.219		Crippen Method
mcvol	229.270	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	1840.00		NIST Webbook
ripol	2364.00		NIST Webbook
tb	622.46	K	Joback Method
tc	797.26	K	Joback Method
tf	301.92	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.25	J/molxK	622.46	Joback Method
cpg	621.33	J/molxK	651.59	Joback Method
cpg	637.60	J/molxK	680.73	Joback Method
cpg	653.10	J/molxK	709.86	Joback Method
cpg	667.88	J/molxK	739.00	Joback Method
cpg	681.97	J/molxK	768.13	Joback Method
cpg	695.41	J/molxK	797.26	Joback Method
dvisc	0.0035968	Paxs	301.92	Joback Method

dvisc	0.0013539	Paxs	355.34	Joback Method
dvisc	0.0006579	Paxs	408.77	Joback Method
dvisc	0.0003778	Paxs	462.19	Joback Method
dvisc	0.0002433	Paxs	515.61	Joback Method
dvisc	0.0001702	Paxs	569.04	Joback Method
dvisc	0.0001266	Paxs	622.46	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=R554800&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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