

(6E,8E)-6,8,10-Undecatrien-4-one

Inchi:	InChI=1S/C11H18O/c1-3-5-6-7-8-10-11(12)9-4-2/h5-8H,3-4,9-10H2,1-2H3/b6-5+,8-7+
InchiKey:	ZQNPNAPTTPCBHP-BSWSSELBSA-N
Formula:	C11H18O
SMILES:	CCC=CC=CCC(=O)CCC
Mol. weight [g/mol]:	166.26

Physical Properties

Property code	Value	Unit	Source
gf	73.26	kJ/mol	Joback Method
hf	-148.51	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.268		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1328.00		NIST Webbook
ripol	1899.00		NIST Webbook
tb	513.27	K	Joback Method
tc	700.01	K	Joback Method
tf	253.50	K	Joback Method
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.56	J/mol×K	513.27	Joback Method
cpg	368.13	J/mol×K	544.39	Joback Method
cpg	381.94	J/mol×K	575.52	Joback Method
cpg	395.05	J/mol×K	606.64	Joback Method
cpg	407.47	J/mol×K	637.77	Joback Method
cpg	419.25	J/mol×K	668.89	Joback Method
cpg	430.43	J/mol×K	700.01	Joback Method
dvisc	0.0039020	Paxs	253.50	Joback Method

dvisc	0.0016040	Paxs	296.80	Joback Method
dvisc	0.0008268	Paxs	340.09	Joback Method
dvisc	0.0004950	Paxs	383.38	Joback Method
dvisc	0.0003289	Paxs	426.68	Joback Method
dvisc	0.0002356	Paxs	469.97	Joback Method
dvisc	0.0001786	Paxs	513.27	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=R590886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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