(6E,8E)-6,8,10-Undecatrien-2-one

Inchi: InChI=1S/C11H18O/c1-3-4-5-6-7-8-9-10-11(2)12/h4-7H,3,8-10H2,1-2H3/b5-4+,7-6+
InchiKey: ITFIJUPFLFMZKL-YTXTXJHMSA-N
Formula: C11H18O
SMILES: CCC=CC=CCCCC(C)=O
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	1338.00		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1947.00		NIST Webbook
tb	513.27	K	Joback Method
tc	700.01	K	Joback Method
tf	253.50	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001786	Pa×s	513.27	Joback Method
dvisc	0.0002356	Pa×s	469.97	Joback Method
dvisc	0.0003289	Pa×s	426.68	Joback Method
dvisc	0.0004950	Pa×s	383.38	Joback Method
dvisc	0.0008268	Pa×s	340.09	Joback Method
dvisc	0.0016040	Pa×s	296.80	Joback Method
dvisc	0.0039020	Pa×s	253.50	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=R590871&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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