

2-(3-Pentoxy)-1,3-cyclohexadiene

Inchi:	InChI=1S/C11H18O/c1-3-10(4-2)12-11-8-6-5-7-9-11/h6,8-10H,3-5,7H2,1-2H3
InchiKey:	OYRUAAIPXOFPBU-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	CCC(CC)OC1=CCCC=C1
Mol. weight [g/mol]:	166.26
CAS:	98677-92-0

Physical Properties

Property code	Value	Unit	Source
gf	16.75	kJ/mol	Joback Method
hf	-229.12	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.425		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	500.58	K	Joback Method
tc	703.49	K	Joback Method
tf	246.62	K	Joback Method
vc	0.570	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.68	J/molxK	500.58	Joback Method
cpg	420.39	J/molxK	669.67	Joback Method
cpg	406.48	J/molxK	635.85	Joback Method
cpg	391.77	J/molxK	602.03	Joback Method
cpg	376.25	J/molxK	568.22	Joback Method
cpg	359.89	J/molxK	534.40	Joback Method
cpg	433.53	J/molxK	703.49	Joback Method
dvisc	0.0001757	Paxs	500.58	Joback Method
dvisc	0.0002376	Paxs	458.25	Joback Method

dvisc	0.0003416	Paxs	415.93	Joback Method
dvisc	0.0005334	Paxs	373.60	Joback Method
dvisc	0.0009331	Paxs	331.27	Joback Method
dvisc	0.0019229	Paxs	288.95	Joback Method
dvisc	0.0050791	Paxs	246.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C98677920&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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