

1-(Prop-2-enyloxy)-2-(prop-2-enyl)-4,5-methylenecyclohexane

Other names:	5-Allyl-6-(allyloxy)-1,3-benzodioxole
Inchi:	InChI=1S/C13H14O3/c1-3-5-10-7-12-13(16-9-15-12)8-11(10)14-6-4-2/h3-4,7-8H,1-2,5-6,10H
InchiKey:	UITAOVXQEWVMGA-UHFFFAOYSA-N
Formula:	C13H14O3
SMILES:	C=CCOc1cc2c(cc1CC=C)OCO2
Mol. weight [g/mol]:	218.25
CAS:	259138-58-4

Physical Properties

Property code	Value	Unit	Source
gf	109.00	kJ/mol	Joback Method
hf	-161.75	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.709		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	619.55	K	Joback Method
tc	836.70	K	Joback Method
tf	394.28	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.99	J/molxK	619.55	Joback Method
cpg	438.99	J/molxK	655.74	Joback Method
cpg	452.12	J/molxK	691.93	Joback Method
cpg	464.43	J/molxK	728.13	Joback Method
cpg	475.97	J/molxK	764.32	Joback Method

cpg	486.79	J/molxK	800.51	Joback Method
cpg	496.95	J/molxK	836.70	Joback Method
dvisc	0.0013798	Paxs	394.28	Joback Method
dvisc	0.0009714	Paxs	431.83	Joback Method
dvisc	0.0007234	Paxs	469.37	Joback Method
dvisc	0.0005627	Paxs	506.91	Joback Method
dvisc	0.0004532	Paxs	544.46	Joback Method
dvisc	0.0003753	Paxs	582.00	Joback Method
dvisc	0.0003180	Paxs	619.55	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=C259138584&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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