1-(Prop-2-ynyloxy)-2-(prop-2-ynyl)-4,5-methylened

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,
InchiKey: UITAOVXQEWVMGA-UHFFFAOYSA-N
Formula: C13H14O3
SMILES: C=CCOc1cc2c(cc1CC=C)OCO2
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
hfus	33.95	kJ/mol	Joback Method
logp	2.709		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	569.50	K	Cheméo Relay (1.0)
tf	303.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.99	J/mol×K	619.55	Joback Method
cpg	438.99	J/mol×K	655.74	Joback Method
cpg	452.12	J/mol×K	691.93	Joback Method
cpg	464.43	J/mol×K	728.13	Joback Method
cpg	475.97	J/mol×K	764.32	Joback Method
cpg	486.79	J/mol×K	800.51	Joback Method
cpg	496.95	J/mol×K	836.70	Joback Method
dvisc	0.0013798	Pa×s	394.28	Joback Method
dvisc	0.0009714	Pa×s	431.83	Joback Method
dvisc	0.0007234	Pa×s	469.37	Joback Method
dvisc	0.0005627	Pa×s	506.91	Joback Method
dvisc	0.0004532	Pa×s	544.46	Joback Method
dvisc	0.0003753	Pa×s	582.00	Joback Method

dvisc	0.0003180	Pa×s	619.55	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C259138584&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point