

(R,E)-6-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-4-metho

Inchi:	InChI=1S/C15H14O5/c1-17-11-7-3-5-9-13(11)19-15(16)20-14-10-6-4-8-12(14)18-2/h3-10
InchiKey:	ORUJFMPWKPVXLZ-UHFFFAOYSA-N
Formula:	C15H14O5
SMILES:	COc1ccccc1OC(=O)Oc1ccccc1OC
Mol. weight [g/mol]:	274.27
CAS:	495-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-267.94	kJ/mol	Joback Method
hf	-544.27	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.282		Crippen Method
mcvol	199.740	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2701.30		NIST Webbook
tb	749.47	K	Joback Method
tc	978.94	K	Joback Method
tf	475.54	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.40	J/molxK	749.47	Joback Method
cpg	556.51	J/molxK	787.71	Joback Method
cpg	569.46	J/molxK	825.96	Joback Method
cpg	581.22	J/molxK	864.20	Joback Method
cpg	591.77	J/molxK	902.45	Joback Method
cpg	601.09	J/molxK	940.69	Joback Method
cpg	609.17	J/molxK	978.94	Joback Method
dvisc	0.0004117	Paxs	475.54	Joback Method

dvisc	0.0002635	Paxs	521.20	Joback Method
dvisc	0.0001812	Paxs	566.85	Joback Method
dvisc	0.0001318	Paxs	612.51	Joback Method
dvisc	0.0001002	Paxs	658.16	Joback Method
dvisc	0.0000789	Paxs	703.82	Joback Method
dvisc	0.0000640	Paxs	749.47	Joback Method

Sources

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=C495852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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