

4-Methoxyphenyl 4'-(3-butenyloxy)benzoate

Inchi:	InChI=1S/C18H18O4/c1-3-4-13-21-16-7-5-14(6-8-16)18(19)22-17-11-9-15(20-2)10-12-17
InchiKey:	CXPLNUIZUUBDCU-UHFFFAOYSA-N
Formula:	C18H18O4
SMILES:	<chem>C=CCCOc1ccc(C(=O)Oc2ccc(OC)cc2)cc1</chem>
Mol. weight [g/mol]:	298.33
CAS:	76487-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-49.84	kJ/mol	Joback Method
hf	-348.54	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.869		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
tb	792.37	K	Joback Method
tc	1017.55	K	Joback Method
tf	485.36	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.12	J/molxK	792.37	Joback Method
cpg	716.00	J/molxK	980.02	Joback Method
cpg	706.01	J/molxK	942.49	Joback Method
cpg	694.85	J/molxK	904.96	Joback Method
cpg	682.49	J/molxK	867.43	Joback Method
cpg	668.92	J/molxK	829.90	Joback Method
cpg	724.82	J/molxK	1017.55	Joback Method
dvisc	0.0000612	Paxs	792.37	Joback Method
dvisc	0.0000762	Paxs	741.20	Joback Method

dvisc	0.0000980	Paxs	690.03	Joback Method
dvisc	0.0001313	Paxs	638.87	Joback Method
dvisc	0.0001850	Paxs	587.70	Joback Method
dvisc	0.0002784	Paxs	536.53	Joback Method
dvisc	0.0004564	Paxs	485.36	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=C76487564&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
mccvol:	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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