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: C=CCCOc1ccc(C(=O)Oc2ccc(OC)cc2)cc1
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/mol×K	792.37	Joback Method
cpg	668.92	J/mol×K	829.90	Joback Method
cpg	682.49	J/mol×K	867.43	Joback Method
cpg	694.85	J/mol×K	904.96	Joback Method
cpg	706.01	J/mol×K	942.49	Joback Method
cpg	716.00	J/mol×K	980.02	Joback Method
cpg	724.82	J/mol×K	1017.55	Joback Method
dvisc	0.0004564	Pa×s	485.36	Joback Method
dvisc	0.0002784	Pa×s	536.53	Joback Method

dvisc	0.0001850	Pa×s	587.70	Joback Method
dvisc	0.0001313	Pa×s	638.87	Joback Method
dvisc	0.0000980	Pa×s	690.03	Joback Method
dvisc	0.0000762	Pa×s	741.20	Joback Method
dvisc	0.0000612	Pa×s	792.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76487564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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