(Z)-Benzyl 3-(4-hydroxy-3-methoxyphenyl)acrylate

Inchi: InChI=1S/C17H16O4/c1-20-16-11-13(7-9-15(16)18)8-10-17(19)21-12-14-5-3-2-4-6-14/h2
InchiKey: DZAPHTCUSDTZAT-NTMALXAHSA-N
Formula: C17H16O4
SMILES: COc1cc(C=CC(=O)OCc2ccccc2)ccc1O
Mol. weight [g/mol]: 284.31
CAS: 132336-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-105.87	kJ/mol	Joback Method
hf	-369.73	kJ/mol	Joback Method
hfus	37.44	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.157		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	830.19	K	Joback Method
tc	1071.69	K	Joback Method
tf	547.74	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.82	J/mol×K	830.19	Joback Method
cpg	636.24	J/mol×K	870.44	Joback Method
cpg	648.81	J/mol×K	910.69	Joback Method
cpg	660.61	J/mol×K	950.94	Joback Method
cpg	671.77	J/mol×K	991.19	Joback Method
cpg	682.39	J/mol×K	1031.44	Joback Method
cpg	692.59	J/mol×K	1071.69	Joback Method

dvisc	0.0000827	Pa×s	547.74	Joback Method
dvisc	0.0000407	Pa×s	594.82	Joback Method
dvisc	0.0000222	Pa×s	641.89	Joback Method
dvisc	0.0000132	Pa×s	688.96	Joback Method
dvisc	0.0000084	Pa×s	736.04	Joback Method
dvisc	0.0000056	Pa×s	783.12	Joback Method
dvisc	0.0000039	Pa×s	830.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132336017&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

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