(S)-6-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-4-methoxy

Inchi: InChI=1S/C15H16O5/c1-17-12-7-11(20-15(16)8-12)4-2-10-3-5-13-14(6-10)19-9-18-13/h3
InchiKey: RSIWXFIBHXYNFM-LLVKDONJSA-N
Formula: C15H16O5
SMILES: COC1=CC(=O)OC(CCc2ccc3c(c2)OCO3)C1
Mol. weight [g/mol]: 276.28
CAS: 19902-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-204.14	kJ/mol	Joback Method
hf	-611.49	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	74.38	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.194		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	2571.80		NIST Webbook
rinpol	2571.80		NIST Webbook
tb	785.43	K	Joback Method
tc	1030.55	K	Joback Method
tf	523.27	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.99	J/mol×K	785.43	Joback Method
cpg	616.69	J/mol×K	826.28	Joback Method
cpg	631.03	J/mol×K	867.14	Joback Method
cpg	644.04	J/mol×K	907.99	Joback Method
cpg	655.74	J/mol×K	948.85	Joback Method
cpg	666.16	J/mol×K	989.70	Joback Method
cpg	675.33	J/mol×K	1030.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19902911&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
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