4-((2S,3R)-4-(Benzo[d][1,3]dioxol-5-yl)-2,3-dimethy

Inchi: InChI=1S/C20H24O4/c1-13(8-15-4-6-17(21)19(10-15)22-3)14(2)9-16-5-7-18-20(11-16)24
InchiKey: QDDILOVMGWUNGD-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: COc1cc(CC(C)C(C)Cc2ccc3c(c2)OCO3)ccc1O
Mol. weight [g/mol]: 328.40
CAS: 107534-93-0

Physical Properties

Property code	Value	Unit	Source
gf	-54.83	kJ/mol	Joback Method
hf	-508.43	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.187		Crippen Method
mcvol	257.760	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2687.70		NIST Webbook
rinpol	2687.70		NIST Webbook
tb	892.77	K	Joback Method
tc	1130.31	K	Joback Method
tf	584.83	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.86	J/mol×K	892.77	Joback Method
cpg	833.68	J/mol×K	932.36	Joback Method
cpg	848.76	J/mol×K	971.95	Joback Method
cpg	863.27	J/mol×K	1011.54	Joback Method
cpg	877.33	J/mol×K	1051.13	Joback Method
cpg	891.10	J/mol×K	1090.72	Joback Method
cpg	904.73	J/mol×K	1130.31	Joback Method

dvisc	0.0001032	Pa×s	584.83	Joback Method
dvisc	0.0000518	Pa×s	636.15	Joback Method
dvisc	0.0000288	Pa×s	687.48	Joback Method
dvisc	0.0000174	Pa×s	738.80	Joback Method
dvisc	0.0000112	Pa×s	790.12	Joback Method
dvisc	0.0000076	Pa×s	841.45	Joback Method
dvisc	0.0000054	Pa×s	892.77	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=C107534930&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