(3R,4R)-3-(Benzo[d][1,3]dioxol-5-ylmethyl)-4-((7-m

Inchi: InChI=1S/C21H20O7/c1-23-18-7-13(8-19-20(18)28-11-27-19)4-14-9-24-21(22)15(14)5-1
InchiKey: GBQHDHMFTXPYAM-CABCVRRESA-N
Formula: C21H20O7
SMILES: COc1cc(CC2COC(=O)C2Cc2ccc3c(c2)OCO3)cc2c1OCO2
Mol. weight [g/mol]: 384.38
CAS: 944284-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-189.82	kJ/mol	Joback Method
hf	-764.56	kJ/mol	Joback Method
hfus	66.01	kJ/mol	Joback Method
hvap	99.80	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	2.727		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	3265.40		NIST Webbook
tb	1016.56	K	Joback Method
tc	1275.56	K	Joback Method
tf	716.19	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.17	J/mol×K	1016.56	Joback Method
cpg	920.14	J/mol×K	1059.73	Joback Method
cpg	931.82	J/mol×K	1102.89	Joback Method
cpg	942.33	J/mol×K	1146.06	Joback Method
cpg	951.76	J/mol×K	1189.23	Joback Method
cpg	960.23	J/mol×K	1232.39	Joback Method
cpg	967.84	J/mol×K	1275.56	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=C944284564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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https://www.chemeo.com/cid/77-490-3/3R-4R-3-Benzo-d-1-3-dioxol-5-ylmethyl-4-7-methoxybenzo-d-1-3-dioxol-5-yl-r
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