

2-Bromo-4,5-dimethoxyphenylacetic acid

Inchi:	InChI=1S/C10H11BrO4/c1-14-8-3-6(4-10(12)13)7(11)5-9(8)15-2/h3,5H,4H2,1-2H3,(H,12
InchiKey:	MDOLAGJJKZEHHW-UHFFFAOYSA-N
Formula:	C10H11BrO4
SMILES:	COc1cc(Br)c(CC(=O)O)cc1OC
Mol. weight [g/mol]:	275.10
CAS:	4697-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-344.58	kJ/mol	Joback Method
hf	-550.53	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.093		Crippen Method
mcvol	164.680	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	726.87	K	Joback Method
tc	937.08	K	Joback Method
tf	481.45	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.22	J/molxK	726.87	Joback Method
cpg	444.86	J/molxK	902.04	Joback Method
cpg	437.77	J/molxK	867.01	Joback Method
cpg	430.05	J/molxK	831.97	Joback Method
cpg	421.72	J/molxK	796.94	Joback Method
cpg	412.78	J/molxK	761.90	Joback Method
cpg	451.32	J/molxK	937.08	Joback Method
dvisc	0.0000370	Paxs	726.87	Joback Method
dvisc	0.0000498	Paxs	685.97	Joback Method

dvisc	0.0000696	Paxs	645.06	Joback Method
dvisc	0.0001018	Paxs	604.16	Joback Method
dvisc	0.0001574	Paxs	563.26	Joback Method
dvisc	0.0002606	Paxs	522.35	Joback Method
dvisc	0.0004701	Paxs	481.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4697625&Units=SI

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

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