Methyl 3,5-dibromo-2,4-dimethoxy-6-methylbenzoate

Inchi: InChI=1S/C11H12Br2O4/c1-5-6(11(14)17-4)9(15-2)8(13)10(16-3)7(5)12/h1-4H3
InchiKey: HCKWDQNSOKQKEN-UHFFFAOYSA-N
Formula: C11H12Br2O4
SMILES: COC(=O)c1c(C)c(Br)c(OC)c(Br)c1OC
Mol. weight [g/mol]: 368.02
CAS: 150965-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-309.28	kJ/mol	Joback Method
hf	-547.77	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	72.51	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.324		Crippen Method
mcvol	196.270	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
tb	756.11	K	Joback Method
tc	987.03	K	Joback Method
tf	538.97	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.61	J/mol×K	756.11	Joback Method
cpg	471.50	J/mol×K	794.60	Joback Method
cpg	481.62	J/mol×K	833.08	Joback Method
cpg	490.93	J/mol×K	871.57	Joback Method
cpg	499.40	J/mol×K	910.06	Joback Method
cpg	507.00	J/mol×K	948.54	Joback Method
cpg	513.71	J/mol×K	987.03	Joback Method
dvisc	0.0003339	Pa×s	538.97	Joback Method
dvisc	0.0002551	Pa×s	575.16	Joback Method

dvisc	0.0002013	Pa×s	611.35	Joback Method
dvisc	0.0001630	Pa×s	647.54	Joback Method
dvisc	0.0001350	Pa×s	683.73	Joback Method
dvisc	0.0001140	Pa×s	719.92	Joback Method
dvisc	0.0000978	Pa×s	756.11	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=C150965734&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume