methyl 2,5-diiodobenzoate

Inchi: InChI=1S/C8H6I2O2/c1-12-8(11)6-4-5(9)2-3-7(6)10/h2-4H,1H3
InchiKey: DYYAKMJJKVLJFN-UHFFFAOYSA-N
Formula: C8H6I2O2
SMILES: COC(=O)c1cc(I)ccc1I
Mol. weight [g/mol]: 387.94

Physical Properties

Property code	Value	Unit	Source
gf	-8.05	kJ/mol	Joback Method
hf	-85.92	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	2.682		Crippen Method
mcvol	158.900	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
tb	681.65	K	Joback Method
tc	965.17	K	Joback Method
tf	419.66	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.54	J/mol×K	681.65	Joback Method
cpg	297.23	J/mol×K	728.90	Joback Method
cpg	305.13	J/mol×K	776.16	Joback Method
cpg	312.28	J/mol×K	823.41	Joback Method
cpg	318.75	J/mol×K	870.66	Joback Method
cpg	324.58	J/mol×K	917.92	Joback Method
cpg	329.81	J/mol×K	965.17	Joback Method
dvisc	0.0013981	Pa×s	419.66	Joback Method

dvisc	0.0008776	Pa×s	463.32	Joback Method
dvisc	0.0005968	Pa×s	506.99	Joback Method
dvisc	0.0004315	Pa×s	550.65	Joback Method
dvisc	0.0003272	Pa×s	594.32	Joback Method
dvisc	0.0002577	Pa×s	637.98	Joback Method
dvisc	0.0002093	Pa×s	681.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389349&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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