

Methyl 3,5-dibromobenzoate

Other names:	Benzoic acid, 3,5-dibromo-, methyl ester
Inchi:	InChI=1S/C8H6Br2O2/c1-12-8(11)5-2-6(9)4-7(10)3-5/h2-4H,1H3
InchiKey:	GSMAWUZTAIOCL-UHFFFAOYSA-N
Formula:	C8H6Br2O2
SMILES:	COC(=O)c1cc(Br)cc(Br)c1
Mol. weight [g/mol]:	293.94
CAS:	51329-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-95.65	kJ/mol	Joback Method
hf	-187.00	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.998		Crippen Method
mcvol	142.260	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	627.69	K	Joback Method
tc	878.22	K	Joback Method
tf	423.14	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.61	J/molxK	627.69	Joback Method
cpg	283.58	J/molxK	669.45	Joback Method
cpg	291.87	J/molxK	711.20	Joback Method
cpg	299.53	J/molxK	752.96	Joback Method
cpg	306.56	J/molxK	794.71	Joback Method
cpg	313.01	J/molxK	836.47	Joback Method
cpg	318.89	J/molxK	878.22	Joback Method

dvisc	0.0010566	Paxs	423.14	Joback Method
dvisc	0.0007517	Paxs	457.23	Joback Method
dvisc	0.0005606	Paxs	491.32	Joback Method
dvisc	0.0004344	Paxs	525.41	Joback Method
dvisc	0.0003472	Paxs	559.51	Joback Method
dvisc	0.0002847	Paxs	593.60	Joback Method
dvisc	0.0002385	Paxs	627.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51329158&Units=SI
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

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

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