Benzene, 1,3-dibromo-2-methoxy-

Other names: 2,6-Dibromoanisole
Inchi: InChI=1S/C7H6Br2O/c1-10-7-5(8)3-2-4-6(7)9/h2-4H,1H3
InchiKey: BMZVDHQOAJUZJL-UHFFFAOYSA-N
Formula: C7H6Br2O
SMILES: COc1c(Br)cccc1Br
Mol. weight [g/mol]: 265.93
CAS: 38603-09-7

Physical Properties

Property code	Value	Unit	Source
gf	24.85	kJ/mol	Joback Method
hf	-53.78	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.220		Crippen Method
mcvol	126.600	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	550.94	K	Joback Method
tc	799.62	K	Joback Method
tf	361.94	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.27	J/mol×K	550.94	Joback Method
cpg	232.27	J/mol×K	592.39	Joback Method
cpg	240.67	J/mol×K	633.83	Joback Method
cpg	248.48	J/mol×K	675.28	Joback Method
cpg	255.74	J/mol×K	716.73	Joback Method
cpg	262.46	J/mol×K	758.18	Joback Method

cpg	268.69	J/mol×K	799.62	Joback Method
dvisc	0.0011466	Pa×s	361.94	Joback Method
dvisc	0.0008062	Pa×s	393.44	Joback Method
dvisc	0.0005973	Pa×s	424.94	Joback Method
dvisc	0.0004612	Pa×s	456.44	Joback Method
dvisc	0.0003682	Pa×s	487.94	Joback Method
dvisc	0.0003021	Pa×s	519.44	Joback Method
dvisc	0.0002535	Pa×s	550.94	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=C38603097&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
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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