Benzene, 2,4-dibromo-1-methoxy-

Other names: 2,4-Dibromoanisole
Inchi: InChI=1S/C7H6Br2O/c1-10-7-3-2-5(8)4-6(7)9/h2-4H,1H3
InchiKey: XGXUGXPKRBQINS-UHFFFAOYSA-N
Formula: C7H6Br2O
SMILES: COc1ccc(Br)cc1Br
Mol. weight [g/mol]: 265.93
CAS: 21702-84-1

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	1448.00		NIST Webbook
rinpol	1448.00		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	262.46	J/mol×K	758.18	Joback Method
cpg	255.74	J/mol×K	716.73	Joback Method
cpg	248.48	J/mol×K	675.28	Joback Method
cpg	240.67	J/mol×K	633.83	Joback Method
cpg	232.27	J/mol×K	592.39	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21702841&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume