1,2-Dibromo-4,5-methylenedioxybenzene

Inchi: InChI=1S/C7H4Br2O2/c8-4-1-6-7(2-5(4)9)11-3-10-6/h1-2H,3H2
InchiKey: WPYAICCSYGUFTK-UHFFFAOYSA-N
Formula: C7H4Br2O2
SMILES: Brc1cc2c(cc1Br)OCO2
Mol. weight [g/mol]: 279.91
CAS: 5279-32-3

Physical Properties

Property code	Value	Unit	Source
gf	16.44	kJ/mol	Joback Method
hf	-103.89	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	2.940		Crippen Method
mcvol	121.610	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
tb	598.81	K	Joback Method
tc	864.82	K	Joback Method
tf	427.55	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.16	J/mol×K	598.81	Joback Method
cpg	263.46	J/mol×K	820.49	Joback Method
cpg	258.07	J/mol×K	776.15	Joback Method
cpg	252.25	J/mol×K	731.82	Joback Method
cpg	245.89	J/mol×K	687.48	Joback Method
cpg	238.90	J/mol×K	643.15	Joback Method
cpg	268.53	J/mol×K	864.82	Joback Method
dvisc	0.0005966	Pa×s	598.81	Joback Method
dvisc	0.0006822	Pa×s	570.27	Joback Method

dvisc	0.0007912	Pa×s	541.72	Joback Method
dvisc	0.0009329	Pa×s	513.18	Joback Method
dvisc	0.0011215	Pa×s	484.64	Joback Method
dvisc	0.0013797	Pa×s	456.09	Joback Method
dvisc	0.0017448	Pa×s	427.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5279323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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