2,6-Dibromo-3,5-dichloroanisole

Inchi: InChI=1S/C7H4Br2Cl2O/c1-12-7-5(8)3(10)2-4(11)6(7)9/h2H,1H3
InchiKey: KLYZBTSHILXGNE-UHFFFAOYSA-N
Formula: C7H4Br2Cl2O
SMILES: COc1c(Br)c(Cl)cc(Cl)c1Br
Mol. weight [g/mol]: 334.82

Physical Properties

Property code	Value	Unit	Source
gf	-18.27	kJ/mol	Joback Method
hf	-108.20	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	60.15	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.527		Crippen Method
mcvol	151.080	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	635.76	K	Joback Method
tc	893.38	K	Joback Method
tf	446.82	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.95	J/mol×K	635.76	Joback Method
cpg	288.32	J/mol×K	850.44	Joback Method
cpg	283.17	J/mol×K	807.51	Joback Method
cpg	277.57	J/mol×K	764.57	Joback Method
cpg	271.51	J/mol×K	721.63	Joback Method
cpg	264.97	J/mol×K	678.70	Joback Method
cpg	293.03	J/mol×K	893.38	Joback Method
dvisc	0.0002123	Pa×s	635.76	Joback Method

dvisc	0.0002467	Pa×s	604.27	Joback Method
dvisc	0.0002915	Pa×s	572.78	Joback Method
dvisc	0.0003511	Pa×s	541.29	Joback Method
dvisc	0.0004327	Pa×s	509.80	Joback Method
dvisc	0.0005483	Pa×s	478.31	Joback Method
dvisc	0.0007182	Pa×s	446.82	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=R323532&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