

2,4-Dibromo-5,6-dichloroanisole

Inchi:	InChI=1S/C7H4Br2Cl2O/c1-12-7-4(9)2-3(8)5(10)6(7)11/h2H,1H3
InchiKey:	MUUDTVDSRYEMBU-UHFFFAOYSA-N
Formula:	C7H4Br2Cl2O
SMILES:	COc1c(Br)cc(Br)c(Cl)c1Cl
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	1734.00		NIST Webbook
rinpol	1734.00		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/molxK	635.76	Joback Method
cpg	288.32	J/molxK	850.44	Joback Method
cpg	283.17	J/molxK	807.51	Joback Method
cpg	277.57	J/molxK	764.57	Joback Method
cpg	271.51	J/molxK	721.63	Joback Method
cpg	264.97	J/molxK	678.70	Joback Method
cpg	293.03	J/molxK	893.38	Joback Method
dvisc	0.0002123	Paxs	635.76	Joback Method

dvisc	0.0002467	Paxs	604.27	Joback Method
dvisc	0.0002915	Paxs	572.78	Joback Method
dvisc	0.0003511	Paxs	541.29	Joback Method
dvisc	0.0004327	Paxs	509.80	Joback Method
dvisc	0.0005483	Paxs	478.31	Joback Method
dvisc	0.0007182	Paxs	446.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323512&Units=SI

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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