

6-Bromo-2,3,4-trichloroanisole

Inchi:	InChI=1S/C7H4BrCl3O/c1-12-7-3(8)2-4(9)5(10)6(7)11/h2H,1H3
InchiKey:	FMCSUKUWLYOGLL-UHFFFAOYSA-N
Formula:	C7H4BrCl3O
SMILES:	COc1c(Br)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	290.37

Physical Properties

Property code	Value	Unit	Source
gf	-44.52	kJ/mol	Joback Method
hf	-150.27	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.418		Crippen Method
mcvol	145.820	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
tb	607.03	K	Joback Method
tc	855.20	K	Joback Method
tf	416.94	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.78	J/molxK	607.03	Joback Method
cpg	283.35	J/molxK	813.84	Joback Method
cpg	277.94	J/molxK	772.48	Joback Method
cpg	272.08	J/molxK	731.11	Joback Method
cpg	265.77	J/molxK	689.75	Joback Method
cpg	259.00	J/molxK	648.39	Joback Method
cpg	288.31	J/molxK	855.20	Joback Method
dvisc	0.0002190	Paxs	607.03	Joback Method

dvisc	0.0002560	Paxs	575.35	Joback Method
dvisc	0.0003046	Paxs	543.67	Joback Method
dvisc	0.0003705	Paxs	511.99	Joback Method
dvisc	0.0004623	Paxs	480.30	Joback Method
dvisc	0.0005952	Paxs	448.62	Joback Method
dvisc	0.0007963	Paxs	416.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R323676&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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