

2,6-Dibromo-4-methoxytoluene

Other names:	Anisole, 3,5-dibromo-4-methyl- 3,5-dibromo-4-methylanisole
Inchi:	InChI=1S/C8H8Br2O/c1-5-7(9)3-6(11-2)4-8(5)10/h3-4H,1-2H3
InchiKey:	BZRKRRXRNGVEIZ-UHFFFAOYSA-N
Formula:	C8H8Br2O
SMILES:	COc1cc(Br)c(C)c(Br)c1
Mol. weight [g/mol]:	279.96
CAS:	14542-71-3

Physical Properties

Property code	Value	Unit	Source
gf	23.64	kJ/mol	Joback Method
hf	-85.89	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.529		Crippen Method
mcvol	140.690	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	578.80	K	Joback Method
tc	823.29	K	Joback Method
tf	385.73	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.05	J/molxK	578.80	Joback Method
cpg	275.00	J/molxK	619.55	Joback Method
cpg	284.33	J/molxK	660.30	Joback Method
cpg	293.08	J/molxK	701.04	Joback Method
cpg	301.25	J/molxK	741.79	Joback Method
cpg	308.88	J/molxK	782.54	Joback Method
cpg	315.97	J/molxK	823.29	Joback Method

dvisc	0.0009260	Paxs	385.73	Joback Method
dvisc	0.0006682	Paxs	417.91	Joback Method
dvisc	0.0005051	Paxs	450.09	Joback Method
dvisc	0.0003964	Paxs	482.26	Joback Method
dvisc	0.0003207	Paxs	514.44	Joback Method
dvisc	0.0002659	Paxs	546.62	Joback Method
dvisc	0.0002252	Paxs	578.80	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=C14542713&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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