2,4,5-Tribromoanisole

Inchi: InChI=1S/C7H5Br3O/c1-11-7-3-5(9)4(8)2-6(7)10/h2-3H,1H3
InchiKey: VHOBLUDHUKOSAT-UHFFFAOYSA-N
Formula: C7H5Br3O
SMILES: COc1cc(Br)c(Br)cc1Br
Mol. weight [g/mol]: 344.83

Physical Properties

Property code	Value	Unit	Source
gf	29.54	kJ/mol	Joback Method
hf	-38.92	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	3.983		Crippen Method
mcvol	144.100	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	622.08	K	Joback Method
tc	885.53	K	Joback Method
tf	434.26	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.12	J/mol×K	622.08	Joback Method
cpg	255.87	J/mol×K	665.99	Joback Method
cpg	263.04	J/mol×K	709.90	Joback Method
cpg	269.68	J/mol×K	753.80	Joback Method
cpg	275.81	J/mol×K	797.71	Joback Method
cpg	281.46	J/mol×K	841.62	Joback Method
cpg	286.69	J/mol×K	885.53	Joback Method
dvisc	0.0008008	Pa×s	434.26	Joback Method

dvisc	0.0006036	Pa×s	465.56	Joback Method
dvisc	0.0004715	Pa×s	496.87	Joback Method
dvisc	0.0003792	Pa×s	528.17	Joback Method
dvisc	0.0003125	Pa×s	559.47	Joback Method
dvisc	0.0002629	Pa×s	590.78	Joback Method
dvisc	0.0002250	Pa×s	622.08	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=R323483&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
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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