

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006036	Paxs	465.56	Joback Method
dvisc	0.0004715	Paxs	496.87	Joback Method
dvisc	0.0003792	Paxs	528.17	Joback Method
dvisc	0.0003125	Paxs	559.47	Joback Method
dvisc	0.0002629	Paxs	590.78	Joback Method
dvisc	0.0002250	Paxs	622.08	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=R323483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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