2,4,6-Tribromo-3-methylphenol

Other names: 2,4,6-Tribromo-3-methylphenol
Phenol, 2,4,6-tribromo-3-methyl-
m-Cresol, 2,4,6-tribromo-
Micatex
Triphysan
Triphysol

Inchi: InChI=1S/C7H5Br3O/c1-3-4(8)2-5(9)7(11)6(3)10/h2,11H,1H3

InchiKey: QKHROXOPRBWBDD-UHFFFAOYSA-N

Formula: C7H5Br3O

SMILES: Cc1c(Br)cc(Br)c(O)c1Br

Mol. weight [g/mol]: 344.83

Physical Properties

Property code	Value	Unit	Source
hf	-28.78	kJ/mol	Cheméo Relay (1.0)
hfs	-131.00 ± 5.00	kJ/mol	NIST Webbook
hfus	28.40	kJ/mol	Joback Method
logp	3.988		Crippen Method
mcvol	144.100	ml/mol	McGowan Method
tf	383.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.16	J/mol×K	680.28	Joback Method
cpg	296.53	J/mol×K	956.37	Joback Method
cpg	290.63	J/mol×K	910.36	Joback Method
cpg	284.94	J/mol×K	864.34	Joback Method
cpg	279.29	J/mol×K	818.33	Joback Method
cpg	273.55	J/mol×K	772.31	Joback Method
cpg	267.55	J/mol×K	726.30	Joback Method
dvisc	0.0000648	Pa×s	602.01	Joback Method
dvisc	0.0000289	Pa×s	680.28	Joback Method
dvisc	0.0000371	Pa×s	654.19	Joback Method

dvisc	0.0000484	Pa×s	628.10	Joback Method
dvisc	0.0001845	Pa×s	523.75	Joback Method
dvisc	0.0000890	Pa×s	575.93	Joback Method
dvisc	0.0001259	Pa×s	549.84	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4619743&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point