2,4,5-Tribromotoluene

Other names: 2,4,5-Tribromotoluene
Inchi: InChI=1S/C7H5Br3/c1-4-2-6(9)7(10)3-5(4)8/h2-3H,1H3
InchiKey: KZZJNNUPNNBCCH-UHFFFAOYSA-N
Formula: C7H5Br3
SMILES: Cc1cc(Br)c(Br)cc1Br
Mol. weight [g/mol]: 328.83

Physical Properties

Property code	Value	Unit	Source
hfus	22.62	kJ/mol	Joback Method
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-5.91		Cheméo Relay (1.0)
logp	4.283		Crippen Method
mcvol	138.230	ml/mol	McGowan Method
tb	559.69	K	Cheméo Relay (1.0)
tf	345.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.22	J/mol×K	599.66	Joback Method
cpg	266.22	J/mol×K	868.00	Joback Method
cpg	261.03	J/mol×K	823.28	Joback Method
cpg	255.47	J/mol×K	778.55	Joback Method
cpg	249.48	J/mol×K	733.83	Joback Method
cpg	242.99	J/mol×K	689.11	Joback Method
cpg	235.92	J/mol×K	644.38	Joback Method
dvisc	0.0004868	Pa×s	505.84	Joback Method
dvisc	0.0002874	Pa×s	599.66	Joback Method
dvisc	0.0003360	Pa×s	568.39	Joback Method
dvisc	0.0004001	Pa×s	537.12	Joback Method
dvisc	0.0010479	Pa×s	412.03	Joback Method
dvisc	0.0006077	Pa×s	474.57	Joback Method
dvisc	0.0007828	Pa×s	443.30	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3278884&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point