PHENOL, 2,4,6-TRIBROMO-, ACETATE

Other names: Acetic acid, 2,4,6-tribromophenyl ester
2,4,6-tribromophenyl acetate
Inchi: InChI=1S/C8H5Br3O2/c1-4(12)13-8-6(10)2-5(9)3-7(8)11/h2-3H,1H3
InchiKey: SLENHFBXWIEZCY-UHFFFAOYSA-N
Formula: C8H5Br3O2
SMILES: CC(=O)Oc1c(Br)cc(Br)cc1Br
Mol. weight [g/mol]: 372.84

Physical Properties

Property code	Value	Unit	Source
hfus	27.99	kJ/mol	Joback Method
ie	8.38	eV	Cheméo Relay (1.0)
logp	3.899		Crippen Method
mcvol	159.760	ml/mol	McGowan Method
tb	560.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.10	J/mol×K	698.83	Joback Method
cpg	305.73	J/mol×K	742.62	Joback Method
cpg	312.73	J/mol×K	786.42	Joback Method
cpg	319.14	J/mol×K	830.21	Joback Method
cpg	325.00	J/mol×K	874.00	Joback Method
cpg	330.36	J/mol×K	917.79	Joback Method
cpg	335.23	J/mol×K	961.59	Joback Method
dvisc	0.0007215	Pa×s	495.46	Joback Method
dvisc	0.0005453	Pa×s	529.36	Joback Method
dvisc	0.0004263	Pa×s	563.25	Joback Method
dvisc	0.0003427	Pa×s	597.14	Joback Method
dvisc	0.0002820	Pa×s	631.04	Joback Method
dvisc	0.0002368	Pa×s	664.93	Joback Method
dvisc	0.0002022	Pa×s	698.83	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=C607954&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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature