2,4,6-Tribromo-3-methylphenyl acetate

Other names: 2,4,6-Tribromo-3-acetyloxytoluene
2,4,6-Tribromo-m-cresol acetate
Inchi: InChI=1S/C9H7Br3O2/c1-4-6(10)3-7(11)9(8(4)12)14-5(2)13/h3H,1-2H3
InchiKey: BRPUKPYVNVKWCE-UHFFFAOYSA-N
Formula: C9H7Br3O2
SMILES: CC(=O)Oc1c(Br)cc(Br)c(C)c1Br
Mol. weight [g/mol]: 386.86

Physical Properties

Property code	Value	Unit	Source
gf	-92.17	kJ/mol	Joback Method
hf	-204.25	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	69.01	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.208		Crippen Method
mcvol	173.850	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpol	1944.00		NIST Webbook
tb	726.69	K	Joback Method
tc	984.06	K	Joback Method
tf	519.25	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.91	J/mol×K	726.69	Joback Method
cpg	380.19	J/mol×K	941.16	Joback Method
cpg	374.10	J/mol×K	898.27	Joback Method
cpg	367.46	J/mol×K	855.37	Joback Method
cpg	360.23	J/mol×K	812.48	Joback Method
cpg	352.39	J/mol×K	769.58	Joback Method
cpg	385.75	J/mol×K	984.06	Joback Method

dvisc	0.0001779	Pa×s	726.69	Joback Method
dvisc	0.0002071	Pa×s	692.12	Joback Method
dvisc	0.0002449	Pa×s	657.54	Joback Method
dvisc	0.0002951	Pa×s	622.97	Joback Method
dvisc	0.0003635	Pa×s	588.40	Joback Method
dvisc	0.0004594	Pa×s	553.82	Joback Method
dvisc	0.0005992	Pa×s	519.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U373456&Units=SI

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