2,4,6-tribromo-3-methylphenyl trifluoroacetate

Other names: 2,4,6-Tribromo-3-trifluoroacetyloxytoluene
2,4,6-Tribromo-m-cresol trifluoroacetate
Inchi: InChI=1S/C9H4Br3F3O2/c1-3-4(10)2-5(11)7(6(3)12)17-8(16)9(13,14)15/h2H,1H3
InchiKey: AOOXTTARAUMVQT-UHFFFAOYSA-N
Formula: C9H4Br3F3O2
SMILES: Cc1c(Br)cc(Br)c(OC(=O)C(F)(F)F)c1Br
Mol. weight [g/mol]: 440.83

Physical Properties

Property code	Value	Unit	Source
gf	-673.76	kJ/mol	Joback Method
hf	-801.33	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	65.27	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.750		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1660.00		NIST Webbook
tb	721.27	K	Joback Method
tc	958.77	K	Joback Method
tf	523.44	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.16	J/mol×K	721.27	Joback Method
cpg	378.29	J/mol×K	760.85	Joback Method
cpg	384.80	J/mol×K	800.44	Joback Method
cpg	390.77	J/mol×K	840.02	Joback Method
cpg	396.23	J/mol×K	879.60	Joback Method
cpg	401.26	J/mol×K	919.18	Joback Method
cpg	405.89	J/mol×K	958.77	Joback Method

Sources

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=U373437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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