Acetic acid, tribromo, 1,1-dimethylethyl ester

Inchi: InChI=1S/C6H9Br3O2/c1-5(2,3)11-4(10)6(7,8)9/h1-3H3
InchiKey: NNWAVDRLTUJGLU-UHFFFAOYSA-N
Formula: C6H9Br3O2
SMILES: CC(C)(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-185.64	kJ/mol	Joback Method
hf	-350.48	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.167		Crippen Method
mcvol	155.340	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
tb	604.99	K	Joback Method
tc	856.30	K	Joback Method
tf	413.78	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.72	J/mol×K	604.99	Joback Method
cpg	343.56	J/mol×K	814.42	Joback Method
cpg	337.39	J/mol×K	772.53	Joback Method
cpg	330.63	J/mol×K	730.65	Joback Method
cpg	323.17	J/mol×K	688.76	Joback Method
cpg	314.90	J/mol×K	646.88	Joback Method
cpg	349.25	J/mol×K	856.30	Joback Method
dvisc	0.0002105	Pa×s	604.99	Joback Method

dvisc	0.0002668	Pa×s	573.12	Joback Method
dvisc	0.0003478	Pa×s	541.25	Joback Method
dvisc	0.0004686	Pa×s	509.38	Joback Method
dvisc	0.0006570	Pa×s	477.52	Joback Method
dvisc	0.0009667	Pa×s	445.65	Joback Method
dvisc	0.0015096	Pa×s	413.78	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=R115772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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