Acetic acid, tribromo, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C7H11Br3O2/c1-4-6(2,3)12-5(11)7(8,9)10/h4H2,1-3H3
InchiKey: YOEDAVKZAFEGPU-UHFFFAOYSA-N
Formula: C7H11Br3O2
SMILES: CCC(C)(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 366.87

Physical Properties

Property code	Value	Unit	Source
gf	-177.22	kJ/mol	Joback Method
hf	-371.12	kJ/mol	Joback Method
hfus	17.70	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.557		Crippen Method
mcvol	169.430	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	1428.00		NIST Webbook
tb	627.87	K	Joback Method
tc	873.60	K	Joback Method
tf	425.05	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.09	J/mol×K	627.87	Joback Method
cpg	361.19	J/mol×K	668.83	Joback Method
cpg	370.37	J/mol×K	709.78	Joback Method
cpg	378.74	J/mol×K	750.74	Joback Method
cpg	386.39	J/mol×K	791.69	Joback Method
cpg	393.44	J/mol×K	832.65	Joback Method
cpg	399.98	J/mol×K	873.60	Joback Method
dvisc	0.0013608	Pa×s	425.05	Joback Method
dvisc	0.0008562	Pa×s	458.85	Joback Method

dvisc	0.0005741	Pa×s	492.66	Joback Method
dvisc	0.0004052	Pa×s	526.46	Joback Method
dvisc	0.0002983	Pa×s	560.26	Joback Method
dvisc	0.0002273	Pa×s	594.07	Joback Method
dvisc	0.0001784	Pa×s	627.87	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=R115787&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