Acetic acid, dibromo, 1-methylbutyl ester

Inchi: InChI=1S/C7H12Br2O2/c1-3-4-5(2)11-7(10)6(8)9/h5-6H,3-4H2,1-2H3
InchiKey: QSZUKPZHUQQQSA-UHFFFAOYSA-N
Formula: C7H12Br2O2
SMILES: CCCC(C)OC(=O)C(Br)Br
Mol. weight [g/mol]: 287.98

Physical Properties

Property code	Value	Unit	Source
gf	-202.10	kJ/mol	Joback Method
hf	-390.51	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.834		Crippen Method
mcvol	151.930	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1742.00		NIST Webbook
tb	567.29	K	Joback Method
tc	782.01	K	Joback Method
tf	330.41	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.74	J/mol×K	567.29	Joback Method
cpg	323.57	J/mol×K	603.08	Joback Method
cpg	333.79	J/mol×K	638.86	Joback Method
cpg	343.42	J/mol×K	674.65	Joback Method
cpg	352.47	J/mol×K	710.44	Joback Method
cpg	360.97	J/mol×K	746.23	Joback Method

cpg	368.94	J/mol×K	782.01	Joback Method
dvisc	0.0029934	Pa×s	330.41	Joback Method
dvisc	0.0015774	Pa×s	369.89	Joback Method
dvisc	0.0009406	Pa×s	409.37	Joback Method
dvisc	0.0006143	Pa×s	448.85	Joback Method
dvisc	0.0004298	Pa×s	488.33	Joback Method
dvisc	0.0003172	Pa×s	527.81	Joback Method
dvisc	0.0002442	Pa×s	567.29	Joback Method

Sources

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=R115663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume