Propanoic acid, 2,3-dibromo-, butyl ester

Inchi: InChI=1S/C7H12Br2O2/c1-2-3-4-11-7(10)6(9)5-8/h6H,2-5H2,1H3
InchiKey: PTODVLUSMZDXKT-UHFFFAOYSA-N
Formula: C7H12Br2O2
SMILES: CCCCOC(=O)C(Br)CBr
Mol. weight [g/mol]: 287.98
CAS: 21179-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-199.66	kJ/mol	Joback Method
hf	-385.23	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	52.81	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.488		Crippen Method
mcvol	151.930	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1327.00		NIST Webbook
tb	567.73	K	Joback Method
tc	777.95	K	Joback Method
tf	345.41	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.32	J/mol×K	567.73	Joback Method
cpg	322.87	J/mol×K	602.77	Joback Method
cpg	332.84	J/mol×K	637.80	Joback Method
cpg	342.24	J/mol×K	672.84	Joback Method
cpg	351.11	J/mol×K	707.87	Joback Method
cpg	359.46	J/mol×K	742.91	Joback Method
cpg	367.31	J/mol×K	777.95	Joback Method
dvisc	0.0023638	Pa×s	345.41	Joback Method

dvisc	0.0013698	Pa×s	382.46	Joback Method
dvisc	0.0008741	Pa×s	419.52	Joback Method
dvisc	0.0006000	Pa×s	456.57	Joback Method
dvisc	0.0004358	Pa×s	493.62	Joback Method
dvisc	0.0003309	Pa×s	530.68	Joback Method
dvisc	0.0002605	Pa×s	567.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21179486&Units=SI
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

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