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

Inchi: InChI=1S/C6H10Br2O2/c1-2-3-10-6(9)5(8)4-7/h5H,2-4H2,1H3
InchiKey: BQCHXTFYXMLUBX-UHFFFAOYSA-N
Formula: C6H10Br2O2
SMILES: CCCOC(=O)C(Br)CBr
Mol. weight [g/mol]: 273.95
CAS: 79762-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-208.08	kJ/mol	Joback Method
hf	-364.59	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	50.59	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.098		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	544.85	K	Joback Method
tc	758.56	K	Joback Method
tf	334.14	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.48	J/mol×K	544.85	Joback Method
cpg	277.99	J/mol×K	580.47	Joback Method
cpg	286.97	J/mol×K	616.09	Joback Method
cpg	295.44	J/mol×K	651.70	Joback Method
cpg	303.42	J/mol×K	687.32	Joback Method
cpg	310.93	J/mol×K	722.94	Joback Method
cpg	317.98	J/mol×K	758.56	Joback Method

dvisc	0.0025030	Pa×s	334.14	Joback Method
dvisc	0.0014779	Pa×s	369.26	Joback Method
dvisc	0.0009563	Pa×s	404.38	Joback Method
dvisc	0.0006633	Pa×s	439.50	Joback Method
dvisc	0.0004857	Pa×s	474.61	Joback Method
dvisc	0.0003713	Pa×s	509.73	Joback Method
dvisc	0.0002938	Pa×s	544.85	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79762768&Units=SI

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