Propanoic acid, 2,3-dibromo, pentyl ester

Inchi: InChI=1S/C8H14Br2O2/c1-2-3-4-5-12-8(11)7(10)6-9/h7H,2-6H2,1H3
InchiKey: AUNZBTHVNYHFQL-UHFFFAOYSA-N
Formula: C8H14Br2O2
SMILES: CCCCCOC(=O)C(Br)CBr
Mol. weight [g/mol]: 302.00

Physical Properties

Property code	Value	Unit	Source
gf	-191.24	kJ/mol	Joback Method
hf	-405.87	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	55.04	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.878		Crippen Method
mcvol	166.020	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	590.61	K	Joback Method
tc	797.50	K	Joback Method
tf	356.68	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.95	J/mol×K	590.61	Joback Method
cpg	369.41	J/mol×K	625.09	Joback Method
cpg	380.25	J/mol×K	659.57	Joback Method
cpg	390.48	J/mol×K	694.06	Joback Method
cpg	400.13	J/mol×K	728.54	Joback Method
cpg	409.22	J/mol×K	763.02	Joback Method
cpg	417.77	J/mol×K	797.50	Joback Method
dvisc	0.0022142	Pa×s	356.68	Joback Method

dvisc	0.0012604	Pa×s	395.67	Joback Method
dvisc	0.0007938	Pa×s	434.66	Joback Method
dvisc	0.0005395	Pa×s	473.64	Joback Method
dvisc	0.0003889	Pa×s	512.63	Joback Method
dvisc	0.0002935	Pa×s	551.62	Joback Method
dvisc	0.0002300	Pa×s	590.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30228&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