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

Inchi: InChI=1S/C8H14Br2O2/c1-6(2)3-4-12-8(11)7(10)5-9/h6-7H,3-5H2,1-2H3
InchiKey: JMGSCPGYIYOURH-UHFFFAOYSA-N
Formula: C8H14Br2O2
SMILES: CC(C)CCOC(=O)C(Br)CBr
Mol. weight [g/mol]: 302.00

Physical Properties

Property code	Value	Unit	Source
gf	-193.68	kJ/mol	Joback Method
hf	-411.15	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.734		Crippen Method
mcvol	166.020	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1383.00		NIST Webbook
tb	590.17	K	Joback Method
tc	801.33	K	Joback Method
tf	341.68	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.39	J/mol×K	590.17	Joback Method
cpg	410.76	J/mol×K	766.13	Joback Method
cpg	401.52	J/mol×K	730.94	Joback Method
cpg	391.68	J/mol×K	695.75	Joback Method
cpg	381.23	J/mol×K	660.56	Joback Method
cpg	370.14	J/mol×K	625.36	Joback Method
cpg	419.43	J/mol×K	801.33	Joback Method
dvisc	0.0002150	Pa×s	590.17	Joback Method
dvisc	0.0002804	Pa×s	548.75	Joback Method

dvisc	0.0003819	Pa×s	507.34	Joback Method
dvisc	0.0005496	Pa×s	465.92	Joback Method
dvisc	0.0008491	Pa×s	424.51	Joback Method
dvisc	0.0014410	Pa×s	383.10	Joback Method
dvisc	0.0027803	Pa×s	341.68	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=R30193&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

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