Propanoic acid, 2,3-dibromo, hexyl ester

Inchi: InChI=1S/C9H16Br2O2/c1-2-3-4-5-6-13-9(12)8(11)7-10/h8H,2-7H2,1H3
InchiKey: GGMSKCDVFZFTEQ-UHFFFAOYSA-N
Formula: C9H16Br2O2
SMILES: CCCCCCOC(=O)C(Br)CBr
Mol. weight [g/mol]: 316.03

Physical Properties

Property code	Value	Unit	Source
gf	-182.82	kJ/mol	Joback Method
hf	-426.51	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.268		Crippen Method
mcvol	180.110	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	613.49	K	Joback Method
tc	817.27	K	Joback Method
tf	367.95	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.27	J/mol×K	613.49	Joback Method
cpg	417.53	J/mol×K	647.45	Joback Method
cpg	429.13	J/mol×K	681.42	Joback Method
cpg	440.08	J/mol×K	715.38	Joback Method
cpg	450.42	J/mol×K	749.35	Joback Method
cpg	460.16	J/mol×K	783.31	Joback Method
cpg	469.33	J/mol×K	817.27	Joback Method
dvisc	0.0020587	Pa×s	367.95	Joback Method
dvisc	0.0011522	Pa×s	408.87	Joback Method

dvisc	0.0007167	Pa×s	449.80	Joback Method
dvisc	0.0004826	Pa×s	490.72	Joback Method
dvisc	0.0003453	Pa×s	531.64	Joback Method
dvisc	0.0002592	Pa×s	572.57	Joback Method
dvisc	0.0002022	Pa×s	613.49	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=R30214&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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