(Z)-3-Hexen-1-ol, dibromoacetate

Inchi: InChI=1S/C8H12Br2O2/c1-2-3-4-5-6-12-8(11)7(9)10/h3-4,7H,2,5-6H2,1H3/b4-3-
InchiKey: PCZGGCUZYASJQJ-ARJAWSKDSA-N
Formula: C8H12Br2O2
SMILES: CCC=CCCOC(=O)C(Br)Br
Mol. weight [g/mol]: 299.99

Physical Properties

Property code	Value	Unit	Source
gf	-111.02	kJ/mol	Joback Method
hf	-288.65	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.002		Crippen Method
mcvol	161.720	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1433.00		NIST Webbook
ripol	2022.00		NIST Webbook
tb	594.77	K	Joback Method
tc	810.53	K	Joback Method
tf	351.60	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.41	J/mol×K	594.77	Joback Method
cpg	348.21	J/mol×K	630.73	Joback Method
cpg	358.36	J/mol×K	666.69	Joback Method
cpg	367.88	J/mol×K	702.65	Joback Method
cpg	376.81	J/mol×K	738.61	Joback Method
cpg	385.20	J/mol×K	774.57	Joback Method
cpg	393.08	J/mol×K	810.53	Joback Method
dvisc	0.0020487	Pa×s	351.60	Joback Method

dvisc	0.0011328	Pa×s	392.13	Joback Method
dvisc	0.0006999	Pa×s	432.66	Joback Method
dvisc	0.0004696	Pa×s	473.19	Joback Method
dvisc	0.0003356	Pa×s	513.71	Joback Method
dvisc	0.0002519	Pa×s	554.24	Joback Method
dvisc	0.0001966	Pa×s	594.77	Joback Method

Sources

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=R296247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume