

(E)-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-ONEGZZNKSA-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	1427.00		NIST Webbook
ripol	2003.00		NIST Webbook
tb	594.77	K	Joback Method
tc	810.53	K	Joback Method
tf	351.60	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0011328	Paxs	392.13	Joback Method
dvisc	0.0006999	Paxs	432.66	Joback Method
dvisc	0.0004696	Paxs	473.19	Joback Method
dvisc	0.0003356	Paxs	513.71	Joback Method
dvisc	0.0002519	Paxs	554.24	Joback Method
dvisc	0.0001966	Paxs	594.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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