

(E)-3-Hexen-1-ol, bromoacetate

Inchi:	InChI=1S/C8H13BrO2/c1-2-3-4-5-6-11-8(10)7-9/h3-4H,2,5-7H2,1H3/b4-3+
InchiKey:	FTORJGKHTVJLQS-ONEGZZNKSA-N
Formula:	C8H13BrO2
SMILES:	CCC=CCCOC(=O)CBr
Mol. weight [g/mol]:	221.09

Physical Properties

Property code	Value	Unit	Source
gf	-122.90	kJ/mol	Joback Method
hf	-309.70	kJ/mol	Joback Method
hfus	24.75	kJ/mol	Joback Method
hvap	48.95	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.281		Crippen Method
mcvol	144.220	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	529.05	K	Joback Method
tc	727.25	K	Joback Method
tf	306.80	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.89	J/molxK	529.05	Joback Method
cpg	313.29	J/molxK	562.08	Joback Method
cpg	324.10	J/molxK	595.12	Joback Method
cpg	334.36	J/molxK	628.15	Joback Method
cpg	344.08	J/molxK	661.18	Joback Method
cpg	353.29	J/molxK	694.22	Joback Method
cpg	362.00	J/molxK	727.25	Joback Method

dvisc	0.0023389	Paxs	306.80	Joback Method
dvisc	0.0012907	Paxs	343.84	Joback Method
dvisc	0.0007996	Paxs	380.88	Joback Method
dvisc	0.0005392	Paxs	417.92	Joback Method
dvisc	0.0003877	Paxs	454.97	Joback Method
dvisc	0.0002930	Paxs	492.01	Joback Method
dvisc	0.0002303	Paxs	529.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26635&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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