

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

Inchi:	InChI=1S/C8H11Br3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h3-4H,2,5-6H2,1H3/b4-3+
InchiKey:	XQAGGAGAPPBDDP-ONEGZZNKSA-N
Formula:	C8H11Br3O2
SMILES:	CCC=CCCOC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	378.88

Physical Properties

Property code	Value	Unit	Source
gf	-91.42	kJ/mol	Joback Method
hf	-265.79	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	60.53	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.724		Crippen Method
mcvol	179.220	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	1623.00		NIST Webbook
tb	658.14	K	Joback Method
tc	894.37	K	Joback Method
tf	428.82	K	Joback Method
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.86	J/molxK	658.14	Joback Method
cpg	381.61	J/molxK	697.51	Joback Method
cpg	390.59	J/molxK	736.88	Joback Method
cpg	398.91	J/molxK	776.26	Joback Method
cpg	406.63	J/molxK	815.63	Joback Method
cpg	413.87	J/molxK	855.00	Joback Method
cpg	420.69	J/molxK	894.37	Joback Method
dvisc	0.0011471	Paxs	428.82	Joback Method
dvisc	0.0007114	Paxs	467.04	Joback Method

dvisc	0.0004743	Paxs	505.26	Joback Method
dvisc	0.0003348	Paxs	543.48	Joback Method
dvisc	0.0002474	Paxs	581.70	Joback Method
dvisc	0.0001897	Paxs	619.92	Joback Method
dvisc	0.0001501	Paxs	658.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26667&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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