3-Buten-1-ol, tribromoacetate

Inchi: InChI=1S/C6H7Br3O2/c1-2-3-4-11-5(10)6(7,8)9/h2H,1,3-4H2
InchiKey: OXFDEYLWHBTVJU-UHFFFAOYSA-N
Formula: C6H7Br3O2
SMILES: C=CCCOC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 350.83

Physical Properties

Property code	Value	Unit	Source
gf	-100.64	kJ/mol	Joback Method
hf	-216.30	kJ/mol	Joback Method
hfus	21.24	kJ/mol	Joback Method
hvap	55.44	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.944		Crippen Method
mcvol	151.040	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
rinpol	1405.00		NIST Webbook
tb	604.90	K	Joback Method
tc	846.04	K	Joback Method
tf	409.60	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.37	J/mol×K	604.90	Joback Method
cpg	289.25	J/mol×K	645.09	Joback Method
cpg	296.42	J/mol×K	685.28	Joback Method
cpg	302.97	J/mol×K	725.47	Joback Method
cpg	308.96	J/mol×K	765.66	Joback Method
cpg	314.46	J/mol×K	805.85	Joback Method
cpg	319.55	J/mol×K	846.04	Joback Method
dvisc	0.0014834	Pa×s	409.60	Joback Method
dvisc	0.0009859	Pa×s	442.15	Joback Method

dvisc	0.0006929	Pa×s	474.70	Joback Method
dvisc	0.0005096	Pa×s	507.25	Joback Method
dvisc	0.0003889	Pa×s	539.80	Joback Method
dvisc	0.0003061	Pa×s	572.35	Joback Method
dvisc	0.0002472	Pa×s	604.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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