3-Buten-1-ol, dibromoacetate

Inchi: InChI=1S/C6H8Br2O2/c1-2-3-4-10-6(9)5(7)8/h2,5H,1,3-4H2
InchiKey: ZJXLTTXALJPISM-UHFFFAOYSA-N
Formula: C6H8Br2O2
SMILES: C=CCCOC(=O)C(Br)Br
Mol. weight [g/mol]: 271.94

Physical Properties

Property code	Value	Unit	Source
gf	-120.24	kJ/mol	Joback Method
hf	-239.16	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.222		Crippen Method
mcvol	133.540	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
ripol	1818.00		NIST Webbook
tb	541.53	K	Joback Method
tc	759.86	K	Joback Method
tf	332.38	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.78	J/mol×K	541.53	Joback Method
cpg	258.48	J/mol×K	577.92	Joback Method
cpg	266.64	J/mol×K	614.31	Joback Method
cpg	274.29	J/mol×K	650.69	Joback Method
cpg	281.46	J/mol×K	687.08	Joback Method
cpg	288.17	J/mol×K	723.47	Joback Method
cpg	294.44	J/mol×K	759.86	Joback Method

dvisc	0.0024118	Pa×s	332.38	Joback Method
dvisc	0.0014483	Pa×s	367.24	Joback Method
dvisc	0.0009501	Pa×s	402.10	Joback Method
dvisc	0.0006666	Pa×s	436.95	Joback Method
dvisc	0.0004929	Pa×s	471.81	Joback Method
dvisc	0.0003799	Pa×s	506.67	Joback Method
dvisc	0.0003028	Pa×s	541.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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