2-Propyn-1-ol, dibromoacetate

Inchi: InChI=1S/C5H4Br2O2/c1-2-3-9-5(8)4(6)7/h1,4H,3H2
InchiKey: APSASYICDFPGGQ-UHFFFAOYSA-N
Formula: C5H4Br2O2
SMILES: C#CCOC(=O)C(Br)Br
Mol. weight [g/mol]: 255.89

Physical Properties

Property code	Value	Unit	Source
gf	6.57	kJ/mol	Joback Method
hf	-52.05	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.279		Crippen Method
mcvol	115.150	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1965.00		NIST Webbook
tb	512.09	K	Joback Method
tc	746.04	K	Joback Method
tf	369.84	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.41	J/mol×K	512.09	Joback Method
cpg	199.60	J/mol×K	551.08	Joback Method
cpg	205.37	J/mol×K	590.07	Joback Method
cpg	210.71	J/mol×K	629.06	Joback Method
cpg	215.68	J/mol×K	668.06	Joback Method
cpg	220.27	J/mol×K	707.05	Joback Method

cpg	224.54	J/mol×K	746.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26372&Units=SI

Legend

cpg:	Ideal gas heat capacity
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