2-Propy1-ol, bromoacetate

Inchi: InChI=1S/C5H5BrO2/c1-2-3-8-5(7)4-6/h1H,3-4H2
InchiKey: IBTTUWBRHGUTTA-UHFFFAOYSA-N
Formula: C5H5BrO2
SMILES: C#CCOC(=O)CBr
Mol. weight [g/mol]: 177.00

Physical Properties

Property code	Value	Unit	Source
gf	-5.31	kJ/mol	Joback Method
hf	-73.10	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.558		Crippen Method
mcvol	97.650	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1731.00		NIST Webbook
tb	446.37	K	Joback Method
tc	657.88	K	Joback Method
tf	325.04	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.58	J/mol×K	446.37	Joback Method
cpg	174.05	J/mol×K	481.62	Joback Method
cpg	180.18	J/mol×K	516.87	Joback Method
cpg	185.99	J/mol×K	552.13	Joback Method
cpg	191.50	J/mol×K	587.38	Joback Method
cpg	196.70	J/mol×K	622.63	Joback Method

cpg	201.62	J/mol×K	657.88	Joback Method

Sources

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=R26340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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