3-Butenyl bromoacetate

Inchi: InChI=1S/C6H7BrO2/c1-2-3-4-9-6(8)5-7/h1H,3-5H2
InchiKey: KEPUSJCWMJKCFF-UHFFFAOYSA-N
Formula: C6H7BrO2
SMILES: C#CCCOC(=O)CBr
Mol. weight [g/mol]: 191.02

Physical Properties

Property code	Value	Unit	Source
gf	3.11	kJ/mol	Joback Method
hf	-93.74	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	0.948		Crippen Method
mcvol	111.740	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
tb	469.25	K	Joback Method
tc	677.91	K	Joback Method
tf	336.31	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.74	J/mol×K	469.25	Joback Method
cpg	212.66	J/mol×K	504.03	Joback Method
cpg	220.18	J/mol×K	538.80	Joback Method
cpg	227.31	J/mol×K	573.58	Joback Method
cpg	234.06	J/mol×K	608.36	Joback Method
cpg	240.45	J/mol×K	643.14	Joback Method
cpg	246.48	J/mol×K	677.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R595707&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume