Acetic acid, thio-, s-2-bromoethyl ester

Inchi: InChI=1S/C4H7BrOS/c1-4(6)7-3-2-5/h2-3H2,1H3
InchiKey: NYHLAZJBJZRGPV-UHFFFAOYSA-N
Formula: C4H7BrOS
SMILES: CC(=O)SCCBr
Mol. weight [g/mol]: 183.07
CAS: 927-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-98.68	kJ/mol	Joback Method
hf	-170.27	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.661		Crippen Method
mcvol	102.640	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	479.73	K	Joback Method
tc	703.60	K	Joback Method
tf	278.97	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.99	J/mol×K	479.73	Joback Method
cpg	184.76	J/mol×K	517.04	Joback Method
cpg	192.09	J/mol×K	554.35	Joback Method
cpg	199.00	J/mol×K	591.66	Joback Method
cpg	205.51	J/mol×K	628.98	Joback Method
cpg	211.63	J/mol×K	666.29	Joback Method
cpg	217.35	J/mol×K	703.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C927708&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume