Acrylic acid, 2-bromo-, ethyl ester

Inchi: InChI=1S/C5H7BrO2/c1-3-8-5(7)4(2)6/h2-3H2,1H3
InchiKey: UCDOJQCUOURTPS-UHFFFAOYSA-N
Formula: C5H7BrO2
SMILES: C=C(Br)C(=O)OCC
Mol. weight [g/mol]: 179.01
CAS: 5459-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-149.09	kJ/mol	Joback Method
hf	-249.36	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	41.73	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.458		Crippen Method
mcvol	101.950	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	452.81	K	Joback Method
tc	657.81	K	Joback Method
tf	262.35	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.83	J/mol×K	452.81	Joback Method
cpg	187.64	J/mol×K	486.98	Joback Method
cpg	195.07	J/mol×K	521.14	Joback Method
cpg	202.15	J/mol×K	555.31	Joback Method
cpg	208.86	J/mol×K	589.48	Joback Method
cpg	215.24	J/mol×K	623.65	Joback Method
cpg	221.27	J/mol×K	657.81	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=C5459358&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume