1-N-hexasulfonyl-3-bromo-2-propanone

Inchi: InChI=1S/C9H17BrO3S/c1-2-3-4-5-6-14(12,13)8-9(11)7-10/h2-8H2,1H3
InchiKey: AVBZQDBKXORQFM-UHFFFAOYSA-N
Formula: C9H17BrO3S
SMILES: CCCCCCS(=O)(=O)CC(=O)CBr
Mol. weight [g/mol]: 285.20
CAS: 90676-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-558.24	kJ/mol	Joback Method
hf	-768.69	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.946		Crippen Method
mcvol	184.830	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	573.13	K	Joback Method
tc	756.98	K	Joback Method
tf	339.48	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.92	J/mol×K	573.13	Joback Method
cpg	436.08	J/mol×K	603.77	Joback Method
cpg	448.59	J/mol×K	634.41	Joback Method
cpg	460.46	J/mol×K	665.06	Joback Method
cpg	471.69	J/mol×K	695.70	Joback Method
cpg	482.30	J/mol×K	726.34	Joback Method
cpg	492.29	J/mol×K	756.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90676009&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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