1-N-pentylsulfonyl-3-bromo-2-propanone

Inchi: InChI=1S/C8H15BrO3S/c1-2-3-4-5-13(11,12)7-8(10)6-9/h2-7H2,1H3
InchiKey: PMMSTPZKUSQIAA-UHFFFAOYSA-N
Formula: C8H15BrO3S
SMILES: CCCCCS(=O)(=O)CC(=O)CBr
Mol. weight [g/mol]: 271.17
CAS: 116402-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-566.66	kJ/mol	Joback Method
hf	-748.05	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.555		Crippen Method
mcvol	170.740	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	550.25	K	Joback Method
tc	736.09	K	Joback Method
tf	328.21	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.78	J/mol×K	550.25	Joback Method
cpg	388.19	J/mol×K	581.22	Joback Method
cpg	399.99	J/mol×K	612.20	Joback Method
cpg	411.19	J/mol×K	643.17	Joback Method
cpg	421.80	J/mol×K	674.14	Joback Method
cpg	431.81	J/mol×K	705.12	Joback Method
cpg	441.25	J/mol×K	736.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402687&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