N-(2-Bromobutyryl)-4-chloro-benzenesulfonamide

Inchi: InChI=1S/C10H11BrClNO3S/c1-2-9(11)10(14)13-17(15,16)8-5-3-7(12)4-6-8/h3-6,9H,2H2
InchiKey: JSTSRHVJJDTSLL-UHFFFAOYSA-N
Formula: C10H11BrClNO3S
SMILES: CCC(Br)C(=O)NS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 340.62
CAS: 301195-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-372.02	kJ/mol	Joback Method
hf	-531.82	kJ/mol	Joback Method
hfus	39.34	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.318		Crippen Method
mcvol	197.380	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	2177.00		NIST Webbook
tb	714.83	K	Joback Method
tc	941.49	K	Joback Method
tf	457.27	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.52	J/mol×K	714.83	Joback Method
cpg	476.65	J/mol×K	752.61	Joback Method
cpg	486.80	J/mol×K	790.38	Joback Method
cpg	496.00	J/mol×K	828.16	Joback Method
cpg	504.28	J/mol×K	865.94	Joback Method
cpg	511.67	J/mol×K	903.71	Joback Method
cpg	518.21	J/mol×K	941.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C301195108&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume