Butyl benzenesulfonate

Other names: Benzenesulfonic acid, butyl ester
Inchi: InChI=1S/C10H14O3S/c1-2-3-9-13-14(11,12)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3
InchiKey: NIKBCKTWWPVAIC-UHFFFAOYSA-N
Formula: C10H14O3S
SMILES: CCCCOS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 214.28
CAS: 80-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-427.81	kJ/mol	Joback Method
hf	-598.77	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	61.17	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.192		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1682.00		NIST Webbook
tb	525.08	K	Joback Method
tc	721.91	K	Joback Method
tf	289.67	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.37	J/mol×K	525.08	Joback Method
cpg	376.22	J/mol×K	557.89	Joback Method
cpg	390.33	J/mol×K	590.69	Joback Method
cpg	403.69	J/mol×K	623.50	Joback Method
cpg	416.30	J/mol×K	656.30	Joback Method
cpg	428.17	J/mol×K	689.11	Joback Method
cpg	439.30	J/mol×K	721.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80444&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume