Benzenesulfonamide, 4-methyl-N-ethyl-N-butyl-

Inchi: InChI=1S/C13H21NO2S/c1-4-6-11-14(5-2)17(15,16)13-9-7-12(3)8-10-13/h7-10H,4-6,11H

InchiKey: CYNQPLYBFFTOKF-UHFFFAOYSA-N

Formula: C13H21NO2S

SMILES: CCCCN(CC)S(=O)(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 255.38

Physical Properties

Property code	Value	Unit	Source
gf	-196.40	kJ/mol	Joback Method
hf	-472.41	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	68.15	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.806		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	588.72	K	Joback Method
tc	778.33	K	Joback Method
tf	346.24	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.00	J/mol×K	588.72	Joback Method
cpg	535.32	J/mol×K	620.32	Joback Method
cpg	551.69	J/mol×K	651.92	Joback Method
cpg	567.13	J/mol×K	683.53	Joback Method
cpg	581.67	J/mol×K	715.13	Joback Method
cpg	595.33	J/mol×K	746.73	Joback Method
cpg	608.13	J/mol×K	778.33	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=U415273&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume