Benzenesulfonamide, 4-methyl-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C13H21NO2S/c1-5-14(10-11(2)3)17(15,16)13-8-6-12(4)7-9-13/h6-9,11H,5,10H

InchiKey: YRYKEXZBFSZSMB-UHFFFAOYSA-N

Formula: C13H21NO2S

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

Mol. weight [g/mol]: 255.38

Physical Properties

Property code	Value	Unit	Source
gf	-198.84	kJ/mol	Joback Method
hf	-477.69	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.662		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
tb	588.28	K	Joback Method
tc	781.51	K	Joback Method
tf	331.24	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.35	J/mol×K	588.28	Joback Method
cpg	536.05	J/mol×K	620.49	Joback Method
cpg	552.75	J/mol×K	652.69	Joback Method
cpg	568.49	J/mol×K	684.90	Joback Method
cpg	583.28	J/mol×K	717.10	Joback Method
cpg	597.15	J/mol×K	749.31	Joback Method
cpg	610.12	J/mol×K	781.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415272&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