

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

Inchi:	InChI=1S/C10H15NO2S/c1-4-11(3)14(12,13)10-7-5-9(2)6-8-10/h5-8H,4H2,1-3H3
InchiKey:	BMSQWPVGLOCPKB-UHFFFAOYSA-N
Formula:	C10H15NO2S
SMILES:	CCN(C)S(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	213.30

Physical Properties

Property code	Value	Unit	Source
gf	-221.66	kJ/mol	Joback Method
hf	-410.49	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.635		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpola	1952.00		NIST Webbook
rinpola	1952.00		NIST Webbook
tb	520.08	K	Joback Method
tc	717.06	K	Joback Method
tf	312.43	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.65	J/mol×K	520.08	Joback Method
cpg	386.21	J/mol×K	552.91	Joback Method
cpg	400.93	J/mol×K	585.74	Joback Method
cpg	414.81	J/mol×K	618.57	Joback Method
cpg	427.88	J/mol×K	651.40	Joback Method
cpg	440.15	J/mol×K	684.23	Joback Method
cpg	451.64	J/mol×K	717.06	Joback Method

Sources

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=U415269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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