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

Inchi: InChI=1S/C18H31NO2S/c1-4-6-7-8-9-10-11-16-19(5-2)22(20,21)18-14-12-17(3)13-15-18

InchiKey: ZJMGPZYTZBUGSC-UHFFFAOYSA-N

Formula: C18H31NO2S

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

Mol. weight [g/mol]: 325.51

Physical Properties

Property code	Value	Unit	Source
gf	-154.30	kJ/mol	Joback Method
hf	-575.61	kJ/mol	Joback Method
hfus	50.43	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.756		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	703.12	K	Joback Method
tc	885.64	K	Joback Method
tf	402.59	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.90	J/mol×K	703.12	Joback Method
cpg	810.75	J/mol×K	733.54	Joback Method
cpg	828.53	J/mol×K	763.96	Joback Method
cpg	845.28	J/mol×K	794.38	Joback Method
cpg	861.02	J/mol×K	824.80	Joback Method
cpg	875.79	J/mol×K	855.22	Joback Method
cpg	889.62	J/mol×K	885.64	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=U415279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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