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

Inchi: InChI=1S/C12H19NO2S/c1-4-10-13(5-2)16(14,15)12-8-6-11(3)7-9-12/h6-9H,4-5,10H2,1-

InchiKey: HXHQLUVCZUZJND-UHFFFAOYSA-N

Formula: C12H19NO2S

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

Mol. weight [g/mol]: 241.35

Physical Properties

Property code	Value	Unit	Source
gf	-204.82	kJ/mol	Joback Method
hf	-451.77	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.416		Crippen Method
mcvol	194.250	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	565.84	K	Joback Method
tc	757.75	K	Joback Method
tf	334.97	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.28	J/mol×K	565.84	Joback Method
cpg	484.11	J/mol×K	597.82	Joback Method
cpg	500.01	J/mol×K	629.81	Joback Method
cpg	515.02	J/mol×K	661.79	Joback Method
cpg	529.16	J/mol×K	693.78	Joback Method
cpg	542.43	J/mol×K	725.76	Joback Method
cpg	554.87	J/mol×K	757.75	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=U415271&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