

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

Inchi: InChI=1S/C23H41NO2S/c1-4-6-7-8-9-10-11-12-13-14-15-16-21-24(5-2)27(25,26)23-19-1
InchiKey: CRNBHQFZMJYQIZ-UHFFFAOYSA-N
Formula: C23H41NO2S
SMILES: CCCCCCCCCCCCCCN(CC)S(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 395.64

Physical Properties

Property code	Value	Unit	Source
gf	-112.20	kJ/mol	Joback Method
hf	-678.81	kJ/mol	Joback Method
hfus	63.38	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.707		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	817.52	K	Joback Method
tc	1004.84	K	Joback Method
tf	458.94	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.85	J/mol×K	817.52	Joback Method
cpg	1111.78	J/mol×K	848.74	Joback Method
cpg	1130.47	J/mol×K	879.96	Joback Method
cpg	1147.97	J/mol×K	911.18	Joback Method
cpg	1164.32	J/mol×K	942.40	Joback Method
cpg	1179.57	J/mol×K	973.62	Joback Method
cpg	1193.75	J/mol×K	1004.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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