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

Inchi: InChI=1S/C16H27NO2S/c1-4-6-7-8-9-14-17(5-2)20(18,19)16-12-10-15(3)11-13-16/h10-1

InchiKey: ISNMRCPNELMWEZ-UHFFFAOYSA-N

Formula: C16H27NO2S

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

Mol. weight [g/mol]: 297.46

Physical Properties

Property code	Value	Unit	Source
gf	-171.14	kJ/mol	Joback Method
hf	-534.33	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	74.83	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.976		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	657.36	K	Joback Method
tc	841.64	K	Joback Method
tf	380.05	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.65	J/mol×K	657.36	Joback Method
cpg	697.02	J/mol×K	688.07	Joback Method
cpg	714.36	J/mol×K	718.79	Joback Method
cpg	730.72	J/mol×K	749.50	Joback Method
cpg	746.11	J/mol×K	780.21	Joback Method
cpg	760.56	J/mol×K	810.93	Joback Method
cpg	774.11	J/mol×K	841.64	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=U415278&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