Benzenesulphonic acid, 4-(5-undecyl)-, methyl ester

Inchi: InChI=1S/C18H30O3S/c1-4-6-8-9-11-16(10-7-5-2)17-12-14-18(15-13-17)22(19,20)21-3/h

InchiKey: APCTYQARZLLBLU-UHFFFAOYSA-N

Formula: C18H30O3S

SMILES: CCCCCCC(CCCC)c1ccc(S(=O)(=O)OC)cc1

Mol. weight [g/mol]: 326.49

Physical Properties

Property code	Value	Unit	Source
gf	-372.52	kJ/mol	Joback Method
hf	-780.64	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.266		Crippen Method
mcvol	274.680	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2372.00		NIST Webbook
tb	712.66	K	Joback Method
tc	898.55	K	Joback Method
tf	377.35	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.69	J/mol×K	712.66	Joback Method
cpg	800.29	J/mol×K	743.64	Joback Method
cpg	817.83	J/mol×K	774.62	Joback Method
cpg	834.31	J/mol×K	805.61	Joback Method
cpg	849.76	J/mol×K	836.59	Joback Method
cpg	864.18	J/mol×K	867.57	Joback Method
cpg	877.60	J/mol×K	898.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U376680&Units=SI

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