Benzenesulphonic acid, 4-(4-dodecyl)-, methyl ester

Inchi: InChI=1S/C19H32O3S/c1-4-6-7-8-9-10-12-17(11-5-2)18-13-15-19(16-14-18)23(20,21)22

InchiKey: SJOZQVLUGPLBPT-UHFFFAOYSA-N

Formula: C19H32O3S

SMILES: CCCCCCCCC(CCC)c1ccc(S(=O)(=O)OC)cc1

Mol. weight [g/mol]: 340.52

Physical Properties

Property code	Value	Unit	Source
gf	-364.10	kJ/mol	Joback Method
hf	-801.28	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.656		Crippen Method
mcvol	288.770	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	735.54	K	Joback Method
tc	921.06	K	Joback Method
tf	388.62	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.80	J/mol×K	735.54	Joback Method
cpg	858.61	J/mol×K	766.46	Joback Method
cpg	876.32	J/mol×K	797.38	Joback Method
cpg	892.95	J/mol×K	828.30	Joback Method
cpg	908.50	J/mol×K	859.22	Joback Method
cpg	923.00	J/mol×K	890.14	Joback Method
cpg	936.46	J/mol×K	921.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376684&Units=SI
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

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