Benzenesulphonic acid, 4-(3-tridecyl)-, methyl ester

Inchi: InChI=1S/C20H34O3S/c1-4-6-7-8-9-10-11-12-13-18(5-2)19-14-16-20(17-15-19)24(21,22
InchiKey: JOXLEGFVGUSTHZ-UHFFFAOYSA-N
Formula: C20H34O3S
SMILES: CCCCCCCCCCC(CC)c1ccc(S(=O)(=O)OC)cc1
Mol. weight [g/mol]: 354.55

Physical Properties

Property code	Value	Unit	Source
gf	-355.68	kJ/mol	Joback Method
hf	-821.92	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.046		Crippen Method
mcvol	302.860	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	758.42	K	Joback Method
tc	944.10	K	Joback Method
tf	399.89	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.87	J/mol×K	758.42	Joback Method
cpg	917.88	J/mol×K	789.37	Joback Method
cpg	935.74	J/mol×K	820.31	Joback Method
cpg	952.48	J/mol×K	851.26	Joback Method
cpg	968.11	J/mol×K	882.21	Joback Method
cpg	982.66	J/mol×K	913.15	Joback Method
cpg	996.14	J/mol×K	944.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376687&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