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

Inchi: InChI=1S/C17H28O3S/c1-4-6-8-10-15(9-7-5-2)16-11-13-17(14-12-16)21(18,19)20-3/h11
InchiKey: HMENQKHRLYCEAC-UHFFFAOYSA-N
Formula: C17H28O3S
SMILES: CCCCCC(CCCC)c1ccc(S(=O)(=O)OC)cc1
Mol. weight [g/mol]: 312.47

Physical Properties

Property code	Value	Unit	Source
gf	-380.94	kJ/mol	Joback Method
hf	-760.00	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.876		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2273.00		NIST Webbook
tb	689.78	K	Joback Method
tc	876.53	K	Joback Method
tf	366.08	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.61	J/mol×K	689.78	Joback Method
cpg	742.98	J/mol×K	720.90	Joback Method
cpg	760.31	J/mol×K	752.03	Joback Method
cpg	776.63	J/mol×K	783.15	Joback Method
cpg	791.94	J/mol×K	814.28	Joback Method
cpg	806.25	J/mol×K	845.40	Joback Method
cpg	819.58	J/mol×K	876.53	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=U376678&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