Sulfonyl bis(p,p'-benzoic acid) 5-hydroxy pentyl ester

Inchi: InChI=1S/C24H30O8S/c25-15-3-1-5-17-31-23(27)19-7-11-21(12-8-19)33(29,30)22-13-9-

InchiKey: SHLVXOQSMQFIJT-UHFFFAOYSA-N

Formula: C24H30O8S

SMILES: O=C(OCCCCCO)c1ccc(S(=O)(=O)c2ccc(C(=O)OCCCCCO)cc2)cc1

Mol. weight [g/mol]: 478.56

CAS: 102955-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-853.26	kJ/mol	Joback Method
hf	-1335.98	kJ/mol	Joback Method
hfus	70.35	kJ/mol	Joback Method
hvap	145.20	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.158		Crippen Method
mcvol	356.210	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
tb	1196.56	K	Joback Method
tc	1494.72	K	Joback Method
tf	742.64	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.59	J/mol×K	1196.56	Joback Method
cpg	1184.69	J/mol×K	1246.25	Joback Method
cpg	1186.04	J/mol×K	1295.95	Joback Method
cpg	1184.72	J/mol×K	1345.64	Joback Method
cpg	1180.81	J/mol×K	1395.33	Joback Method
cpg	1174.39	J/mol×K	1445.03	Joback Method
cpg	1165.53	J/mol×K	1494.72	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=C102955135&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume