Sulfonyl-o,p'-diphenacyldibenzoate

Inchi: InChI=1S/C30H22O8S/c31-27(21-9-3-1-4-10-21)19-37-29(33)23-13-7-15-25(17-23)39(35
InchiKey: OLGCDFZBUZUSOG-UHFFFAOYSA-N
Formula: C30H22O8S
SMILES: O=C(COC(=O)c1cccc(S(=O)(=O)c2cccc(C(=O)OCC(=O)c3ccccc3)c2)c1)c1ccccc1
Mol. weight [g/mol]: 542.56

Physical Properties

Property code	Value	Unit	Source
gf	-562.12	kJ/mol	Joback Method
hf	-907.46	kJ/mol	Joback Method
hfus	68.99	kJ/mol	Joback Method
hvap	143.24	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	4.599		Crippen Method
mcvol	384.630	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
tb	1310.58	K	Joback Method
tc	1604.95	K	Joback Method
tf	841.32	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.08	J/mol×K	1310.58	Joback Method
cpg	1182.33	J/mol×K	1359.64	Joback Method
cpg	1176.34	J/mol×K	1408.70	Joback Method
cpg	1168.25	J/mol×K	1457.76	Joback Method
cpg	1158.18	J/mol×K	1506.83	Joback Method
cpg	1146.28	J/mol×K	1555.89	Joback Method
cpg	1132.67	J/mol×K	1604.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000045&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume