2-Naphthyl-p-tolyl sulfone

Inchi: InChI=1S/C17H14O2S/c1-13-6-9-16(10-7-13)20(18,19)17-11-8-14-4-2-3-5-15(14)12-17/h
InchiKey: UOUHDIZYOCFQKG-UHFFFAOYSA-N
Formula: C17H14O2S
SMILES: Cc1ccc(S(=O)(=O)c2ccc3ccccc3c2)cc1
Mol. weight [g/mol]: 282.36
CAS: 13250-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-64.07	kJ/mol	Joback Method
hf	-206.37	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.981		Crippen Method
mcvol	211.500	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	718.44	K	Joback Method
tc	963.13	K	Joback Method
tf	427.00 ± 3.00	K	NIST Webbook
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.84	J/mol×K	718.44	Joback Method
cpg	564.56	J/mol×K	759.22	Joback Method
cpg	578.89	J/mol×K	800.00	Joback Method
cpg	591.90	J/mol×K	840.78	Joback Method
cpg	603.68	J/mol×K	881.57	Joback Method
cpg	614.31	J/mol×K	922.35	Joback Method
cpg	623.88	J/mol×K	963.13	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=C13250061&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume