2,2',5,5'-TETRAMETHYLDIPHENYLSULPHONE

Other names: 2,5-Xylyl sulfone
Inchi: InChI=1S/C16H18O2S/c1-11-5-7-13(3)15(9-11)19(17,18)16-10-12(2)6-8-14(16)4/h5-10H
InchiKey: LVRGWIOEAZMJCV-UHFFFAOYSA-N
Formula: C16H18O2S
SMILES: Cc1ccc(C)c(S(=O)(=O)c2cc(C)ccc2C)c1
Mol. weight [g/mol]: 274.38

Physical Properties

Property code	Value	Unit	Source
af	0.6494		Cheméo Relay (1.0)
gf	-198.40	kJ/mol	Joback Method
hf	-237.97	kJ/mol	Cheméo Relay (1.0)
hfus	35.10	kJ/mol	Joback Method
hvap	106.90	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	3.753		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	657.66	K	Cheméo Relay (1.0)
tc	909.03	K	Cheméo Relay (1.0)
tf	416.00 ± 3.00	K	NIST Webbook
vc	0.777	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.18	J/mol×K	686.54	Joback Method
cpg	576.01	J/mol×K	723.87	Joback Method
cpg	591.65	J/mol×K	761.20	Joback Method
cpg	606.12	J/mol×K	798.53	Joback Method
cpg	619.43	J/mol×K	835.86	Joback Method
cpg	631.60	J/mol×K	873.19	Joback Method
cpg	642.67	J/mol×K	910.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6632446&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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