P-TOLYLMETHANETHIOL

Other names: p-Xylene-alpha-thiol
p-xylene-«alpha»-thiol
Inchi: InChI=1S/C8H10S/c1-7-2-4-8(6-9)5-3-7/h2-5,9H,6H2,1H3
InchiKey: AGFYZLVFPSGUIX-UHFFFAOYSA-N
Formula: C8H10S
SMILES: Cc1ccc(CS)cc1
Mol. weight [g/mol]: 138.24

Physical Properties

Property code	Value	Unit	Source
af	0.4268		Cheméo Relay (1.0)
gf	148.65	kJ/mol	Joback Method
hf	41.13	kJ/mol	Cheméo Relay (1.0)
hfus	14.17	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.425		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	481.82	K	Cheméo Relay (1.0)
tc	710.45	K	Cheméo Relay (1.0)
tf	261.65	K	Cheméo Relay (1.0)
vc	0.418	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.48	J/mol×K	476.96	Joback Method
cpg	234.25	J/mol×K	516.37	Joback Method
cpg	246.23	J/mol×K	555.77	Joback Method
cpg	257.43	J/mol×K	595.18	Joback Method
cpg	267.90	J/mol×K	634.58	Joback Method
cpg	277.66	J/mol×K	673.99	Joback Method

cpg	286.76	J/mol×K	713.39	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4498991&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

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