3,4-Dimethylbenzyl isothiocyanate

Inchi: InChI=1S/C10H11NS/c1-8-3-4-10(5-9(8)2)6-11-7-12/h3-5H,6H2,1-2H3
InchiKey: BNOGRVSYSGZCDC-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: Cc1ccc(CN=C=S)cc1C
Mol. weight [g/mol]: 177.27
CAS: 206559-59-3

Physical Properties

Property code	Value	Unit	Source
hf	247.93	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.906		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	610.79	K	Joback Method
tc	861.13	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C206559593&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

hf: Enthalpy of formation 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