4-Methylphenethyl isothiocyanate

Inchi: InChI=1S/C10H11NS/c1-9-2-4-10(5-3-9)6-7-11-8-12/h2-5H,6-7H2,1H3
InchiKey: GLZKGBMKYHSHAI-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: Cc1ccc(CCN=C=S)cc1
Mol. weight [g/mol]: 177.27
CAS: 13203-39-9

Physical Properties

Property code	Value	Unit	Source
hf	259.40	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.640		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	605.81	K	Joback Method
tc	855.14	K	Joback Method

Sources

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=C13203399&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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