4-Decylphenyl isothiocyanate

Inchi: InChI=1S/C17H25NS/c1-2-3-4-5-6-7-8-9-10-16-11-13-17(14-12-16)18-15-19/h11-14H,2-1
InchiKey: KLRFMWXUZQXOFA-UHFFFAOYSA-N
Formula: C17H25NS
SMILES: CCCCCCCCCCc1ccc(N=C=S)cc1
Mol. weight [g/mol]: 275.45
CAS: 206559-54-8

Physical Properties

Property code	Value	Unit	Source
hf	114.92	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.104		Crippen Method
mcvol	244.360	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
tb	765.97	K	Joback Method
tc	984.49	K	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=C206559548&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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