Allylphenylthiourea

Other names: Allylphenylthiourea
Inchi: InChI=1S/C10H12N2S/c1-2-8-11-10(13)12-9-6-4-3-5-7-9/h2-7H,1,8H2,(H2,11,12,13)
InchiKey: RJTICPGQFMYYEG-UHFFFAOYSA-N
Formula: C10H12N2S
SMILES: C=CCNC(=S)Nc1ccccc1
Mol. weight [g/mol]: 192.29

Physical Properties

Property code	Value	Unit	Source
hfus	29.22	kJ/mol	Joback Method
ie	7.78	eV	Cheméo Relay (1.0)
log10ws	-3.56		Cheméo Relay (1.0)
logp	2.159		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
tb	575.12	K	Cheméo Relay (1.0)
tf	358.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.57	J/mol×K	621.94	Joback Method
cpg	378.31	J/mol×K	661.08	Joback Method
cpg	390.04	J/mol×K	700.22	Joback Method
cpg	400.85	J/mol×K	739.36	Joback Method
cpg	410.84	J/mol×K	778.50	Joback Method
cpg	420.13	J/mol×K	817.64	Joback Method
cpg	428.79	J/mol×K	856.78	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C27177328
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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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