3-Carboxyphenyl isothiocyanate

Inchi: InChI=1S/C8H5NO2S/c10-8(11)6-2-1-3-7(4-6)9-5-12/h1-4H,(H,10,11)
InchiKey: PJRBPKOOGLKPFB-UHFFFAOYSA-N
Formula: C8H5NO2S
SMILES: O=C(O)c1cccc(N=C=S)c1
Mol. weight [g/mol]: 179.20

Physical Properties

Property code	Value	Unit	Source
af	0.6693		Cheméo Relay (1.0)
gf	-45.65	kJ/mol	Cheméo Relay (1.0, beta)
hf	-78.36	kJ/mol	Cheméo Relay (1.0)
hvap	93.82	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	-3.08		Cheméo Relay (1.0)
logp	2.119		Crippen Method
mcvol	124.990	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	562.80	K	Cheméo Relay (1.0)
tc	863.71	K	Cheméo Relay (1.0)
tf	445.36	K	Cheméo Relay (1.0)
vc	0.421	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131637&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):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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