

4-Carboxyphenyl isothiocyanate

Inchi:	InChI=1S/C8H5NO2S/c10-8(11)6-1-3-7(4-2-6)9-5-12/h1-4H,(H,10,11)
InchiKey:	RBEFRYQKJYMLCC-UHFFFAOYSA-N
Formula:	C8H5NO2S
SMILES:	O=C(O)c1ccc(N=C=S)cc1
Mol. weight [g/mol]:	179.20

Physical Properties

Property code	Value	Unit	Source
af	0.6772		Cheméo Relay (1.0)
gf	-45.14	kJ/mol	Cheméo Relay (1.0, beta)
hf	-83.17	kJ/mol	Cheméo Relay (1.0)
hvap	95.49	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.119		Crippen Method
mvol	124.990	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	562.83	K	Cheméo Relay (1.0)
tc	856.42	K	Cheméo Relay (1.0)
tf	514.93	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=C2131626&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

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