BENZOYL ISOTHIOCYANATE

Other names:	Benzoic acid, anhydride with isothiocyanic acid
	Benzoic acid, anhydride with HNCS
	Benzoylthiocarbimide
	N-Benzoyl isothiocyanate
	NSC 29259
Inchi:	InChI=1S/C8H5NOS/c10-8(9-6-11)7-4-2-1-3-5-7/h1-5H
InchiKey:	CPEKAXYCDKETEN-UHFFFAOYSA-N
Formula:	C8H5NOS
SMILES:	O=C(N=C=S)c1ccccc1
Mol. weight [g/mol]:	163.20

Physical Properties

Property code	Value	Unit	Source
af	0.4192		Cheméo Relay (1.0)
gf	143.17	kJ/mol	Cheméo Relay (1.0, beta)
hf	80.96	kJ/mol	Cheméo Relay (1.0)
hvap	61.12	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-3.04		Cheméo Relay (1.0)
logp	1.930		Crippen Method
mcvol	119.120	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	510.12	K	Cheméo Relay (1.0)
tc	770.72	K	Cheméo Relay (1.0)
tf	305.40	K	Cheméo Relay (1.0)
vc	0.413	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00 ± 2.00	K	2.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C532558&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume