

BENZOYL ISOCYANATE

Other names:	Methanone, 1-phenyl-1-isocyanato-
Inchi:	InChI=1S/C8H5NO2/c10-6-9-8(11)7-4-2-1-3-5-7/h1-5H
InchiKey:	LURYMYITPCOQAU-UHFFFAOYSA-N
Formula:	C8H5NO2
SMILES:	O=C=NC(=O)c1ccccc1
Mol. weight [g/mol]:	147.13

Physical Properties

Property code	Value	Unit	Source
af	0.4828		Cheméo Relay (1.0)
gf	0.63	kJ/mol	Cheméo Relay (1.0, beta)
hf	-153.47	kJ/mol	Cheméo Relay (1.0)
hvap	53.33	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	NIST Webbook
log10ws	-2.02		Cheméo Relay (1.0)
logp	1.163		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	490.62	K	Cheméo Relay (1.0)
tc	710.28	K	Cheméo Relay (1.0)
tf	299.00	K	NIST Webbook
vc	0.393	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	475.00	K	96.50	NIST Webbook
tbrp	362.50 ± 1.50	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4461330&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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