

Alpha-benzil, dioxime

Other names:	Benzil, dioxime Dibenzoyl dioxime Diphenyl glyoxime «alpha»-Diphenylglyoxime «alpha»-Benzil dioxime Glyoxime, diphenyl- alpha-Benzil, dioxime 1,2-Diphenyl-1,2-ethanedione dioxime NSC 4042 diphenylethanedione dioxime
Inchi:	InChI=1S/C14H12N2O2/c17-15-13(11-7-3-1-4-8-11)14(16-18)12-9-5-2-6-10-12/h1-10,17
InchiKey:	JJZONEUCDUQVGR-UHFFFAOYSA-N
Formula:	C14H12N2O2
SMILES:	ON=C(C(=NO)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.26

Physical Properties

Property code	Value	Unit	Source
af	0.8716		Cheméo Relay (1.0)
gf	378.89	kJ/mol	Cheméo Relay (1.0, beta)
hf	199.94	kJ/mol	Cheméo Relay (1.0)
hvap	96.67	kJ/mol	Cheméo Relay (1.0)
ie	8.46	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.743		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	611.12	K	Cheméo Relay (1.0)
tc	949.56	K	Cheméo Relay (1.0)
tf	398.08	K	Cheméo Relay (1.0)
vc	0.649	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23873816&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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