

DIETHYL AZODIFORMATE

Other names:	Ethyl azodicarboxylate Diazenedicarboxylic acid, diethyl ester Diethoxycarbonyldiazene Diethyl azodiformate Diethyl diazodicarboxylate Formic acid, azodi-, diethyl ester
Inchi:	InChI=1S/C6H10N2O4/c1-3-11-5(9)7-8-6(10)12-4-2/h3-4H2,1-2H3
InchiKey:	FAMRKDQNMBBFBR-UHFFFAOYSA-N
Formula:	C6H10N2O4
SMILES:	CCOC(=O)N=NC(=O)OCC
Mol. weight [g/mol]:	174.16

Physical Properties

Property code	Value	Unit	Source
af	0.7253		Cheméo Relay (1.0)
gf	-241.55	kJ/mol	Cheméo Relay (1.0, beta)
hf	-613.36	kJ/mol	Cheméo Relay (1.0)
hvap	64.99	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
logp	1.752		Crippen Method
mcvol	125.940	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	488.05	K	Cheméo Relay (1.0)
tc	636.80	K	Cheméo Relay (1.0)
tf	280.73	K	Cheméo Relay (1.0)
vc	0.508	m3/kmol	Cheméo Relay (1.0)

Sources

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):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1972287&Units=SI>

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
h_{vap}:	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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