DIETHYL 4,4'-AZOXYDIBENZOATE

Other names:	Azoxybenzene-4,4'-dicarboxylic acid biethyl ester
	Benzoic acid, 4,4'-azoxybis-, diethyl ester
	Benzoic acid, 4,4'-azoxydi-, diethyl ester
	Diethyl azoxybenzene-4,4'-dicarboxylate
	Diethyl 4,4'-azoxybenzoate
	Diethyl azoxybenzoate
	Diethyl p,p'-azoxybenzoate
	4,4'-Azoxybenzoic acid diethyl ester
	Benzoic acid, 4,4'-(1-oxido-1,2-diazenediyl)bis-, 1,1'-diethyl ester
	Benzoic acid, p,p'-azoxydi-, diethyl ester
	NSC 401032
	diethyl 4,4'-azoxybisbenzoate
	Ethyl azoxybenzenedicarboxylate
Inchi:	InChI=1S/C18H18N2O5/c1-3-24-17(21)13-5-9-15(10-6-13)19-20(23)16-11-7-14(8-12-16)
InchiKey:	LOOVRYZFUGHEMF-UHFFFAOYSA-N
Formula:	C18H18N2O5
SMILES:	CCOC(=O)c1ccc(N=[N+]([O-])c2ccc(C(=O)OCC)cc2)cc1
Mol. weight [g/mol]:	342.35

Physical Properties

Property code	Value	Unit	Source
af	0.9308		Cheméo Relay (1.0)
hf	-430.73	kJ/mol	Cheméo Relay (1.0)
hvap	109.15	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-4.87		Cheméo Relay (1.0)
logp	3.966		Crippen Method
mcvol	253.370	ml/mol	McGowan Method
pc	1693.02	kPa	Cheméo Relay (1.0, beta)
tb	664.81	K	Cheméo Relay (1.0)
tc	942.26	K	Cheméo Relay (1.0)
tf	345.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	451.00	J/mol×K	303.00	NIST Webbook
hfust	20.48	kJ/mol	386.90	NIST Webbook
sfust	52.90	J/mol×K	386.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6421041&Units=SI

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

Legend

af: Acentric Factor
cps: Solid phase heat capacity
hf: Enthalpy of formation at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point