Diethylphthalimidomalonate

Other names:	Diethyl phthalimidomalonate
	Propanedioic acid, (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-, diethyl ester
	Ethyl phthalimidomalonate
	2-Isoindolinemalonic acid, 1,3-dioxo-, diethyl ester
Inchi:	InChI=1S/C15H15NO6/c1-3-21-14(19)11(15(20)22-4-2)16-12(17)9-7-5-6-8-10(9)13(16)18
InchiKey:	SZNGBHWKVWEBKW-UHFFFAOYSA-N
Formula:	C15H15NO6
SMILES:	CCOC(=O)C(C(=O)OCC)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	305.29

Physical Properties

Property code	Value	Unit	Source
af	0.7734		Cheméo Relay (1.0)
hf	-920.43	kJ/mol	Cheméo Relay (1.0)
hvap	94.02	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-3.07		Cheméo Relay (1.0)
logp	0.777		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	1852.69	kPa	Cheméo Relay (1.0, beta)
tb	639.21	K	Cheméo Relay (1.0)
tc	893.47	K	Cheméo Relay (1.0)
tf	383.64	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5680615&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
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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