ETHANEDIOIC ACID, DIPHENYL ESTER

Other names: Ethanedioic acid, diphenyl ester
Oxalic acid, diphenyl ester
Inchi: InChI=1S/C14H10O4/c15-13(17-11-7-3-1-4-8-11)14(16)18-12-9-5-2-6-10-12/h1-10H
InchiKey: ULOZDEVJRTYKFE-UHFFFAOYSA-N
Formula: C14H10O4
SMILES: O=C(Oc1ccccc1)C(=O)Oc1ccccc1
Mol. weight [g/mol]: 242.23

Physical Properties

Property code	Value	Unit	Source
af	0.7034		Cheméo Relay (1.0)
chs	-6399.00 ± 3.00	kJ/mol	NIST Webbook
gf	-176.02	kJ/mol	Joback Method
hf	-437.20 ± 9.20	kJ/mol	NIST Webbook
hfs	-540.00 ± 3.00	kJ/mol	NIST Webbook
hfus	25.67	kJ/mol	Joback Method
hsub	103.00 ± 8.40	kJ/mol	NIST Webbook
hsub	102.80	kJ/mol	NIST Webbook
hvap	93.71	kJ/mol	Cheméo Relay (1.0)
ie	7.94	eV	NIST Webbook
log10ws	-3.83		Cheméo Relay (1.0)
logp	2.198		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	595.78	K	Cheméo Relay (1.0)
tc	857.82	K	Cheméo Relay (1.0)
tf	362.89	K	Cheméo Relay (1.0)
vc	0.652	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.58	J/mol×K	929.38	Joback Method
cpg	514.89	J/mol×K	970.13	Joback Method

cpg	467.35	J/mol×K	766.40	Joback Method
cpg	479.12	J/mol×K	807.15	Joback Method
cpg	489.73	J/mol×K	847.89	Joback Method
cpg	499.20	J/mol×K	888.64	Joback Method
cpg	454.39	J/mol×K	725.66	Joback Method
dvisc	0.0003849	Pa×s	538.35	Joback Method
dvisc	0.0005919	Pa×s	491.53	Joback Method
dvisc	0.0009967	Pa×s	444.70	Joback Method
dvisc	0.0002681	Pa×s	585.18	Joback Method
dvisc	0.0001971	Pa×s	632.01	Joback Method
dvisc	0.0001511	Pa×s	678.83	Joback Method
dvisc	0.0001199	Pa×s	725.66	Joback Method
hfust	31.38	kJ/mol	403.00	NIST Webbook

Sources

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=C3155166&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

hsub: Enthalpy of sublimation 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