BENZENEACETIC ACID, PHENYL ESTER

Other names: Phenylacetic acid, phenyl ester
Inchi: InChI=1S/C14H12O2/c15-14(11-12-7-3-1-4-8-12)16-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey: USVNNHYNCCJCCP-UHFFFAOYSA-N
Formula: C14H12O2
SMILES: O=C(Cc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]: 212.25

Physical Properties

Property code	Value	Unit	Source
af	0.5636		Cheméo Relay (1.0)
hf	-154.94	kJ/mol	Cheméo Relay (1.0)
hfus	22.89	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	2.835		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	574.87	K	Cheméo Relay (1.0)
tc	844.64	K	Cheméo Relay (1.0)
tf	317.83	K	Cheméo Relay (1.0)
vc	0.616	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.95	J/mol×K	649.37	Joback Method
cpg	431.27	J/mol×K	689.83	Joback Method
cpg	445.36	J/mol×K	730.29	Joback Method
cpg	458.28	J/mol×K	770.75	Joback Method
cpg	470.08	J/mol×K	811.21	Joback Method
cpg	480.83	J/mol×K	851.67	Joback Method

cpg	490.57	J/mol×K	892.14	Joback Method
dvisc	0.0016037	Pa×s	372.54	Joback Method
dvisc	0.0008710	Pa×s	418.68	Joback Method
dvisc	0.0005339	Pa×s	464.82	Joback Method
dvisc	0.0003576	Pa×s	510.96	Joback Method
dvisc	0.0002559	Pa×s	557.09	Joback Method
dvisc	0.0001928	Pa×s	603.23	Joback Method
dvisc	0.0001512	Pa×s	649.37	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C722010&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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume