2,2-DIPHENYLPROPIONIC ACID

Other names: «alpha»,«alpha»-Diphenylpropionic acid
Benzeneacetic acid, «alpha»-methyl-«alpha»-phenyl-
Inchi: InChI=1S/C15H14O2/c1-15(14(16)17,12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3,(H
InchiKey: ODELFXJUOVNEFZ-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: CC(C(=O)O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 226.28

Physical Properties

Property code	Value	Unit	Source
af	0.6607		Cheméo Relay (1.0)
gf	37.34	kJ/mol	Joback Method
hf	-229.41	kJ/mol	Cheméo Relay (1.0)
hfus	20.96	kJ/mol	Joback Method
hvap	70.65	kJ/mol	Cheméo Relay (1.0)
ie	8.49	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	3.077		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	590.49	K	Cheméo Relay (1.0)
tc	885.44	K	Cheméo Relay (1.0)
tf	443.72	K	Cheméo Relay (1.0)
vc	0.626	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.73	J/mol×K	738.78	Joback Method
cpg	509.60	J/mol×K	777.73	Joback Method
cpg	521.38	J/mol×K	816.68	Joback Method
cpg	532.18	J/mol×K	855.63	Joback Method
cpg	542.09	J/mol×K	894.58	Joback Method
cpg	551.22	J/mol×K	933.53	Joback Method

cpg	559.68	J/mol×K	972.48	Joback Method
dvisc	0.0016801	Pa×s	424.82	Joback Method
dvisc	0.0005989	Pa×s	477.15	Joback Method
dvisc	0.0002617	Pa×s	529.47	Joback Method
dvisc	0.0001328	Pa×s	581.80	Joback Method
dvisc	0.0000753	Pa×s	634.13	Joback Method
dvisc	0.0000466	Pa×s	686.45	Joback Method
dvisc	0.0000309	Pa×s	738.78	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5558667&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

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume