PHENYLACETIC ACID PROPYL ESTER

Other names:	Benzeneacetic acid, propyl ester
	Acetic acid, phenyl-, propyl ester
	Propyl benzeneacetate
	Propyl phenylacetate
Inchi:	InChI=1S/C11H14O2/c1-2-8-13-11(12)9-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey:	GXXFZZLGPFNITM-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
af	0.5291		Cheméo Relay (1.0)
gf	-79.77	kJ/mol	Joback Method
hf	-342.58	kJ/mol	Cheméo Relay (1.0)
hfus	21.07	kJ/mol	Joback Method
hvap	60.69	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-2.52		Cheméo Relay (1.0)
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1331.02		NIST Webbook
rinpol	1309.25		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1309.25		NIST Webbook
rinpol	1325.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	520.17	K	Cheméo Relay (1.0)
tc	719.13	K	Cheméo Relay (1.0)
tf	246.92	K	Cheméo Relay (1.0)
vc	0.551	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/mol×K	554.05	Joback Method
cpg	421.37	J/mol×K	763.32	Joback Method
cpg	410.76	J/mol×K	728.44	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	387.33	J/mol×K	658.68	Joback Method
cpg	374.48	J/mol×K	623.81	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0002006	Pa×s	554.05	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0012165	Pa×s	352.60	Joback Method

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=C4606159&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume