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
CAS:	4606-15-9

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1309.25		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1331.02		NIST Webbook
rinpol	1309.25		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4606159&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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