2-(Propoxycarbonyl)benzoic acid

Other names: 1,2-Benzenedicarboxylic acid, 1-propyl ester
Propyl hydrogen phthalate
Monopropyl phthalate
Phthalic acid, monopropyl ester
Inchi: InChI=1S/C11H12O4/c1-2-7-15-11(14)9-6-4-3-5-8(9)10(12)13/h3-6H,2,7H2,1H3,(H,12,13
InchiKey: NFOQRIXSEYVCJP-UHFFFAOYSA-N
Formula: C11H12O4
SMILES: CCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	-355.14	kJ/mol	Joback Method
hf	-554.92	kJ/mol	Joback Method
hfus	26.37	kJ/mol	Joback Method
hvap	75.60	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.952		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1731.00		NIST Webbook
tb	705.08	K	Joback Method
tc	908.75	K	Joback Method
tf	435.58	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.52	J/mol×K	705.08	Joback Method
cpg	421.94	J/mol×K	739.02	Joback Method
cpg	431.69	J/mol×K	772.97	Joback Method
cpg	440.78	J/mol×K	806.91	Joback Method
cpg	449.21	J/mol×K	840.86	Joback Method

cpg	457.00	J/mol×K	874.80	Joback Method
cpg	464.18	J/mol×K	908.75	Joback Method
dvisc	0.0012318	Pa×s	435.58	Joback Method
dvisc	0.0005613	Pa×s	480.50	Joback Method
dvisc	0.0002925	Pa×s	525.41	Joback Method
dvisc	0.0001690	Pa×s	570.33	Joback Method
dvisc	0.0001057	Pa×s	615.25	Joback Method
dvisc	0.0000705	Pa×s	660.16	Joback Method
dvisc	0.0000495	Pa×s	705.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume