Benzoic acid, 1-phenylethyl ester

Inchi: InChI=1S/C15H14O2/c1-12(13-8-4-2-5-9-13)17-15(16)14-10-6-3-7-11-14/h2-12H,1H3
InchiKey: NIHKUOHNHOWTCI-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: CC(OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	63.88	kJ/mol	Joback Method
hf	-129.95	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.605		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1744.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2518.00		NIST Webbook
ripol	2530.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2504.00		NIST Webbook
tb	671.81	K	Joback Method
tc	914.44	K	Joback Method
tf	368.81	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.27	J/mol×K	671.81	Joback Method
cpg	535.55	J/mol×K	874.00	Joback Method
cpg	524.26	J/mol×K	833.56	Joback Method
cpg	511.85	J/mol×K	793.13	Joback Method
cpg	498.25	J/mol×K	752.69	Joback Method
cpg	483.41	J/mol×K	712.25	Joback Method
cpg	545.78	J/mol×K	914.44	Joback Method
dvisc	0.0001264	Pa×s	671.81	Joback Method
dvisc	0.0001649	Pa×s	621.31	Joback Method
dvisc	0.0002254	Pa×s	570.81	Joback Method
dvisc	0.0003275	Pa×s	520.31	Joback Method
dvisc	0.0005154	Pa×s	469.81	Joback Method
dvisc	0.0009050	Pa×s	419.31	Joback Method
dvisc	0.0018537	Pa×s	368.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368943&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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