

Benzoic acid, 1-phenylpropyl ester

Inchi:	InChI=1S/C16H16O2/c1-2-15(13-9-5-3-6-10-13)18-16(17)14-11-7-4-8-12-14/h3-12,15H,2
InchiKey:	XCHIHJDABCLLEG-UHFFFAOYSA-N
Formula:	C16H16O2
SMILES:	CCC(OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	72.30	kJ/mol	Joback Method
hf	-150.59	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.995		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpola	1893.00		NIST Webbook
tb	694.69	K	Joback Method
tc	932.29	K	Joback Method
tf	380.08	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.39	J/molxK	694.69	Joback Method
cpg	535.89	J/molxK	734.29	Joback Method
cpg	551.08	J/molxK	773.89	Joback Method
cpg	565.02	J/molxK	813.49	Joback Method
cpg	577.78	J/molxK	853.09	Joback Method
cpg	589.42	J/molxK	892.69	Joback Method
cpg	599.99	J/molxK	932.29	Joback Method
dvisc	0.0017325	Paxs	380.08	Joback Method
dvisc	0.0008345	Paxs	432.52	Joback Method

dvisc	0.0004708	Paxs	484.95	Joback Method
dvisc	0.0002970	Paxs	537.38	Joback Method
dvisc	0.0002033	Paxs	589.82	Joback Method
dvisc	0.0001481	Paxs	642.26	Joback Method
dvisc	0.0001132	Paxs	694.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U368964&Units=SI

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

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