Butanoic acid, phenyl ester

Other names:	Butyric acid, phenyl ester
	Phenyl butyrate
Inchi:	InChI=1S/C10H12O2/c1-2-6-10(11)12-9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3
InchiKey:	IGVPBCZDHMIOJH-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCCC(=O)Oc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	4346-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.392		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1245.00		NIST Webbook
tb	500.65 ± 1.00	K	NIST Webbook
tc	743.85	K	Joback Method
tf	301.04	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.47	J/mol×K	531.17	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method

cpg	370.98	J/mol×K	743.85	Joback Method
dvisc	0.0002164	Pa×s	531.17	Joback Method
dvisc	0.0002757	Pa×s	492.81	Joback Method
dvisc	0.0003660	Pa×s	454.46	Joback Method
dvisc	0.0005118	Pa×s	416.11	Joback Method
dvisc	0.0007662	Pa×s	377.75	Joback Method
dvisc	0.0012567	Pa×s	339.39	Joback Method
dvisc	0.0023380	Pa×s	301.04	Joback Method

Sources

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=C4346183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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