Butyric acid, 2-phenyl-, phenyl ester

Inchi: InChI=1S/C16H16O2/c1-2-15(13-9-5-3-6-10-13)16(17)18-14-11-7-4-8-12-14/h3-12,15H,2
InchiKey: USOFKNJNPHEBDW-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CCC(C(=O)Oc1ccccc1)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	-4.20		Crippen Method
logp	3.786		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
tb	694.69	K	Joback Method
tc	932.29	K	Joback Method
tf	380.08	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.39	J/mol×K	694.69	Joback Method
cpg	535.89	J/mol×K	734.29	Joback Method
cpg	551.08	J/mol×K	773.89	Joback Method
cpg	565.02	J/mol×K	813.49	Joback Method
cpg	577.78	J/mol×K	853.09	Joback Method
cpg	589.42	J/mol×K	892.69	Joback Method
cpg	599.99	J/mol×K	932.29	Joback Method
dvisc	0.0017325	Pa×s	380.08	Joback Method

dvisc	0.0008345	Pa×s	432.52	Joback Method
dvisc	0.0004708	Pa×s	484.95	Joback Method
dvisc	0.0002970	Pa×s	537.38	Joback Method
dvisc	0.0002033	Pa×s	589.82	Joback Method
dvisc	0.0001481	Pa×s	642.26	Joback Method
dvisc	0.0001132	Pa×s	694.69	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=U406872&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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