

Butyric acid, 2-phenyl-, 3-methylphenyl ester

Inchi:	InChI=1S/C17H18O2/c1-3-16(14-9-5-4-6-10-14)17(18)19-15-11-7-8-13(2)12-15/h4-12,16
InchiKey:	GIRKRCYXBLTILP-UHFFFAOYSA-N
Formula:	C17H18O2
SMILES:	CCC(C(=O)Oc1cccc(C)c1)c1ccccc1
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	71.09	kJ/mol	Joback Method
hf	-182.70	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	67.42	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.094		Crippen Method
mvol	210.310	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	722.55	K	Joback Method
tc	956.32	K	Joback Method
tf	403.87	K	Joback Method
vc	0.789	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.89	J/molxK	722.55	Joback Method
cpg	588.49	J/molxK	761.51	Joback Method
cpg	603.83	J/molxK	800.47	Joback Method
cpg	617.93	J/molxK	839.44	Joback Method
cpg	630.87	J/molxK	878.40	Joback Method
cpg	642.70	J/molxK	917.36	Joback Method
cpg	653.47	J/molxK	956.32	Joback Method
dvisc	0.0012874	Paxs	403.87	Joback Method

dvisc	0.0006579	Paxs	456.98	Joback Method
dvisc	0.0003866	Paxs	510.10	Joback Method
dvisc	0.0002512	Paxs	563.21	Joback Method
dvisc	0.0001758	Paxs	616.32	Joback Method
dvisc	0.0001302	Paxs	669.44	Joback Method
dvisc	0.0001008	Paxs	722.55	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=U406873&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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