

Butyric acid, 2-phenyl-, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C23H22O3/c1-2-22(19-11-7-4-8-12-19)23(24)26-21-15-13-20(14-16-21)25-17-
InchiKey:	PIGCRLOQWZAHMD-UHFFFAOYSA-N
Formula:	C23H22O3
SMILES:	CCC(C(=O)O)c1ccc(OCc2ccccc2)cc1)c1ccccc1
Mol. weight [g/mol]:	346.42

Physical Properties

Property code	Value	Unit	Source
gf	129.02	kJ/mol	Joback Method
hf	-202.23	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	85.46	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.365		Crippen Method
mvol	276.960	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2701.00		NIST Webbook
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tb	908.93	K	Joback Method
tc	1153.90	K	Joback Method
tf	520.14	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.17	J/molxK	908.93	Joback Method
cpg	902.10	J/molxK	1113.07	Joback Method
cpg	893.07	J/molxK	1072.24	Joback Method
cpg	882.74	J/molxK	1031.42	Joback Method
cpg	871.04	J/molxK	990.59	Joback Method
cpg	857.87	J/molxK	949.76	Joback Method
cpg	909.92	J/molxK	1153.90	Joback Method
dvisc	0.0000362	Paxs	908.93	Joback Method

dvisc	0.0000468	Paxs	844.13	Joback Method
dvisc	0.0000632	Paxs	779.33	Joback Method
dvisc	0.0000902	Paxs	714.54	Joback Method
dvisc	0.0001382	Paxs	649.74	Joback Method
dvisc	0.0002325	Paxs	584.94	Joback Method
dvisc	0.0004456	Paxs	520.14	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=U406877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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