

Butyric acid, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C17H18O3/c1-2-6-17(18)20-16-11-9-15(10-12-16)19-13-14-7-4-3-5-8-14/h3-5,
InchiKey:	ZOEUZNCAWXZTMB-UHFFFAOYSA-N
Formula:	C17H18O3
SMILES:	CCCC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	270.32

Physical Properties

Property code	Value	Unit	Source
gf	-31.47	kJ/mol	Joback Method
hf	-309.64	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.971		Crippen Method
mvol	216.180	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2148.00		NIST Webbook
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tb	745.41	K	Joback Method
tc	971.98	K	Joback Method
tf	441.10	K	Joback Method
vc	0.814	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.41	J/molxK	745.41	Joback Method
cpg	614.18	J/molxK	783.17	Joback Method
cpg	628.74	J/molxK	820.93	Joback Method
cpg	642.13	J/molxK	858.69	Joback Method
cpg	654.37	J/molxK	896.46	Joback Method
cpg	665.49	J/molxK	934.22	Joback Method
cpg	675.53	J/molxK	971.98	Joback Method
dvisc	0.0007907	Paxs	441.10	Joback Method

dvisc	0.0004493	Paxs	491.82	Joback Method
dvisc	0.0002838	Paxs	542.54	Joback Method
dvisc	0.0001939	Paxs	593.25	Joback Method
dvisc	0.0001407	Paxs	643.97	Joback Method
dvisc	0.0001070	Paxs	694.69	Joback Method
dvisc	0.0000844	Paxs	745.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307520&Units=SI
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

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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