

Butanoic acid, phenylmethyl ester

Other names:	Butyric acid, benzyl ester Benzyl butanoate Benzyl butyrate Benzyl n-butanoate Benzyl n-butyrate n-Butyric acid benzyl ester Benzylester kyseliny maselne Butanoic acid, benzyl ester NSC 8073 Phenylmethyl butanoate Phenylmethyl butyrate
Inchi:	InChI=1S/C11H14O2/c1-2-6-11(12)13-9-10-7-4-3-5-8-10/h3-5,7-8H,2,6,9H2,1H3
InchiKey:	VONGZNXBKCOUHB-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	103-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.530		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1354.50		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1305.00		NIST Webbook

rinpol	1314.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1315.80		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1339.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1311.10		NIST Webbook
rinpol	1312.80		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1863.90		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1865.80		NIST Webbook
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/molxK	554.05	Joback Method
cpg	360.84	J/molxK	588.93	Joback Method
cpg	374.48	J/molxK	623.81	Joback Method
cpg	387.33	J/molxK	658.68	Joback Method
cpg	399.42	J/molxK	693.56	Joback Method
cpg	410.76	J/molxK	728.44	Joback Method
cpg	421.37	J/molxK	763.32	Joback Method
dvisc	0.0023060	Paxs	312.31	Joback Method
dvisc	0.0012165	Paxs	352.60	Joback Method
dvisc	0.0007317	Paxs	392.89	Joback Method
dvisc	0.0004838	Paxs	433.18	Joback Method
dvisc	0.0003432	Paxs	473.47	Joback Method
dvisc	0.0002569	Paxs	513.76	Joback Method
dvisc	0.0002006	Paxs	554.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103377&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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