

Butyric acid, 4-phenyl-, pentyl ester

Inchi:	InChI=1S/C15H22O2/c1-2-3-7-13-17-15(16)12-8-11-14-9-5-4-6-10-14/h4-6,9-10H,2-3,7-8
InchiKey:	ZHTGUNVTDPBJLC-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	-46.09	kJ/mol	Joback Method
hf	-361.20	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.743		Crippen Method
mvol	205.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1741.00		NIST Webbook
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tb	645.57	K	Joback Method
tc	843.08	K	Joback Method
tf	357.39	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.39	J/molxK	645.57	Joback Method
cpg	621.23	J/molxK	810.16	Joback Method
cpg	608.02	J/molxK	777.24	Joback Method
cpg	593.96	J/molxK	744.32	Joback Method
cpg	579.02	J/molxK	711.41	Joback Method
cpg	563.17	J/molxK	678.49	Joback Method
cpg	633.62	J/molxK	843.08	Joback Method
dvisc	0.0001364	Paxs	645.57	Joback Method

dvisc	0.0001776	Paxs	597.54	Joback Method
dvisc	0.0002424	Paxs	549.51	Joback Method
dvisc	0.0003510	Paxs	501.48	Joback Method
dvisc	0.0005498	Paxs	453.45	Joback Method
dvisc	0.0009578	Paxs	405.42	Joback Method
dvisc	0.0019370	Paxs	357.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406174&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
mccvol:	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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