

Butyric acid, 2-phenyl-, pentyl ester

Inchi:	InChI=1S/C15H22O2/c1-3-5-9-12-17-15(16)14(4-2)13-10-7-6-8-11-13/h6-8,10-11,14H,3-
InchiKey:	PDLMYOAIQPIQLF-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	-48.53	kJ/mol	Joback Method
hf	-366.48	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.914		Crippen Method
mvol	205.890	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1570.00		NIST Webbook
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tb	645.13	K	Joback Method
tc	846.21	K	Joback Method
tf	342.39	K	Joback Method
vc	0.785	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.83	J/molxK	645.13	Joback Method
cpg	622.96	J/molxK	812.70	Joback Method
cpg	609.57	J/molxK	779.18	Joback Method
cpg	595.30	J/molxK	745.67	Joback Method
cpg	580.10	J/molxK	712.16	Joback Method
cpg	563.95	J/molxK	678.64	Joback Method
cpg	635.49	J/molxK	846.21	Joback Method
dvisc	0.0001267	Paxs	645.13	Joback Method

dvisc	0.0001684	Paxs	594.67	Joback Method
dvisc	0.0002360	Paxs	544.22	Joback Method
dvisc	0.0003541	Paxs	493.76	Joback Method
dvisc	0.0005830	Paxs	443.30	Joback Method
dvisc	0.0010907	Paxs	392.85	Joback Method
dvisc	0.0024547	Paxs	342.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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