Butyric acid, 2-phenyl-, pent-2-yl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-50.97	kJ/mol	Joback Method
hf	-371.76	kJ/mol	Joback Method
hfus	24.39	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.912		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	644.69	K	Joback Method
tc	849.49	K	Joback Method
tf	327.39	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.27	J/mol×K	644.69	Joback Method
cpg	624.73	J/mol×K	815.35	Joback Method
cpg	611.16	J/mol×K	781.22	Joback Method
cpg	596.67	J/mol×K	747.09	Joback Method
cpg	581.20	J/mol×K	712.96	Joback Method
cpg	564.75	J/mol×K	678.82	Joback Method
cpg	637.40	J/mol×K	849.49	Joback Method
dvisc	0.0001178	Pa×s	644.69	Joback Method

dvisc	0.0001598	Pa×s	591.81	Joback Method
dvisc	0.0002302	Pa×s	538.92	Joback Method
dvisc	0.0003589	Pa×s	486.04	Joback Method
dvisc	0.0006237	Pa×s	433.16	Joback Method
dvisc	0.0012640	Pa×s	380.27	Joback Method
dvisc	0.0032184	Pa×s	327.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406870&Units=SI

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