Butyric acid, 2-phenyl-, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H20O2/c1-4-14(13-8-6-5-7-9-13)15(16)17-11-10-12(2)3/h5-10,14H,4,11H2

InchiKey: CTASMGAMKMQDNO-UHFFFAOYSA-N

Formula: C15H20O2

SMILES: CCC(C(=O)OCC=C(C)C)c1ccccc1

Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	23.14	kJ/mol	Joback Method
hf	-259.05	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.690		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	649.17	K	Joback Method
tc	861.36	K	Joback Method
tf	323.35	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.18	J/mol×K	649.17	Joback Method
cpg	542.06	J/mol×K	684.54	Joback Method
cpg	557.90	J/mol×K	719.90	Joback Method
cpg	572.73	J/mol×K	755.27	Joback Method
cpg	586.62	J/mol×K	790.63	Joback Method
cpg	599.60	J/mol×K	826.00	Joback Method
cpg	611.72	J/mol×K	861.36	Joback Method

Sources

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=U406915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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