Butyric acid, 2-phenyl-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C20H26O2/c1-6-19(17-10-8-7-9-11-17)20(21)22-18(14-16(4)5)13-12-15(2)3/h7

InchiKey: IKZXFTGYQYJYBW-UHFFFAOYSA-N

Formula: C20H26O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)C(CC)c1ccccc1

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	270.78	kJ/mol	Joback Method
hf	-92.30	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	71.94	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.718		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	764.21	K	Joback Method
tc	984.80	K	Joback Method
tf	459.12	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.28	J/mol×K	764.21	Joback Method
cpg	772.67	J/mol×K	800.98	Joback Method
cpg	789.80	J/mol×K	837.74	Joback Method
cpg	805.73	J/mol×K	874.51	Joback Method
cpg	820.53	J/mol×K	911.27	Joback Method
cpg	834.23	J/mol×K	948.04	Joback Method
cpg	846.90	J/mol×K	984.80	Joback Method

Sources

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=U406919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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