Butyric acid, 2-phenyl-, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C19H26O2/c1-5-7-13-17(14-15(3)4)21-19(20)18(6-2)16-11-9-8-10-12-16/h8-12

InchiKey: LOJIOLGLNIGEJX-UHFFFAOYSA-N

Formula: C19H26O2

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

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	183.07	kJ/mol	Joback Method
hf	-187.30	kJ/mol	Joback Method
hfus	34.35	kJ/mol	Joback Method
hvap	70.31	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.552		Crippen Method
mcvol	253.650	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	1853.00		NIST Webbook
tb	744.77	K	Joback Method
tc	961.83	K	Joback Method
tf	463.57	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.15	J/mol×K	744.77	Joback Method
cpg	741.64	J/mol×K	780.95	Joback Method
cpg	758.91	J/mol×K	817.12	Joback Method
cpg	775.00	J/mol×K	853.30	Joback Method
cpg	789.95	J/mol×K	889.47	Joback Method
cpg	803.81	J/mol×K	925.65	Joback Method
cpg	816.62	J/mol×K	961.83	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=U406918&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