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

Inchi: InChI=1S/C19H26O2/c1-4-5-13-18(15-16(2)3)21-19(20)14-9-12-17-10-7-6-8-11-17/h6-8,

InchiKey: RBVDGQJDPPXOLD-UHFFFAOYSA-N

Formula: C19H26O2

SMILES: CCC#CC(CC(C)C)OC(=O)CCCc1ccccc1

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	185.51	kJ/mol	Joback Method
hf	-182.02	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.381		Crippen Method
mcvol	253.650	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	2026.00		NIST Webbook
tb	745.21	K	Joback Method
tc	958.73	K	Joback Method
tf	478.57	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.64	J/mol×K	745.21	Joback Method
cpg	740.82	J/mol×K	780.80	Joback Method
cpg	757.83	J/mol×K	816.38	Joback Method
cpg	773.70	J/mol×K	851.97	Joback Method
cpg	788.49	J/mol×K	887.56	Joback Method
cpg	802.22	J/mol×K	923.15	Joback Method
cpg	814.95	J/mol×K	958.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406986&Units=SI
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

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