Butyric acid, 2-phenyl-, hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H20O2/c1-4-10-14(5-2)18-16(17)15(6-3)13-11-8-7-9-12-13/h7-9,11-12,14-
InchiKey: MVHOLHOUPNQQIJ-UHFFFAOYSA-N
Formula: C16H20O2
SMILES: CC#CC(CC)OC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	160.25	kJ/mol	Joback Method
hf	-120.10	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.525		Crippen Method
mcvol	211.380	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	676.57	K	Joback Method
tc	900.26	K	Joback Method
tf	444.76	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.65	J/mol×K	676.57	Joback Method
cpg	575.07	J/mol×K	713.85	Joback Method
cpg	591.35	J/mol×K	751.13	Joback Method
cpg	606.53	J/mol×K	788.42	Joback Method
cpg	620.66	J/mol×K	825.70	Joback Method
cpg	633.76	J/mol×K	862.98	Joback Method
cpg	645.88	J/mol×K	900.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406916&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

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