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

Inchi: InChI=1S/C16H20O2/c1-3-9-15(4-2)18-16(17)13-8-12-14-10-6-5-7-11-14/h5-7,10-11,15H
InchiKey: NBCNAJHCARHGOQ-UHFFFAOYSA-N
Formula: C16H20O2
SMILES: CC#CC(CC)OC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	162.69	kJ/mol	Joback Method
hf	-114.82	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.354		Crippen Method
mcvol	211.380	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	677.01	K	Joback Method
tc	896.46	K	Joback Method
tf	459.76	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.16	J/mol×K	677.01	Joback Method
cpg	574.21	J/mol×K	713.59	Joback Method
cpg	590.19	J/mol×K	750.16	Joback Method
cpg	605.12	J/mol×K	786.74	Joback Method
cpg	619.04	J/mol×K	823.31	Joback Method
cpg	631.99	J/mol×K	859.89	Joback Method
cpg	644.00	J/mol×K	896.46	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=U406984&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