3-Phenylpropionic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C18H24O2/c1-4-5-11-17(14-15(2)3)20-18(19)13-12-16-9-7-6-8-10-16/h6-10,15

InchiKey: GLIPACJKXJXVPU-UHFFFAOYSA-N

Formula: C18H24O2

SMILES: CCC#CC(CC(C)C)OC(=O)CCc1ccccc1

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	177.09	kJ/mol	Joback Method
hf	-161.38	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.991		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	722.33	K	Joback Method
tc	938.81	K	Joback Method
tf	467.30	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.49	J/mol×K	722.33	Joback Method
cpg	684.48	J/mol×K	758.41	Joback Method
cpg	701.30	J/mol×K	794.49	Joback Method
cpg	717.00	J/mol×K	830.57	Joback Method
cpg	731.62	J/mol×K	866.65	Joback Method
cpg	745.19	J/mol×K	902.73	Joback Method
cpg	757.77	J/mol×K	938.81	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=U299176&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