Phenylacetic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H22O2/c1-4-5-11-16(12-14(2)3)19-17(18)13-15-9-7-6-8-10-15/h6-10,14,16
InchiKey: OPDLFTTWEXFJKN-UHFFFAOYSA-N
Formula: C17H22O2
SMILES: CCC#CC(CC(C)C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
gf	168.67	kJ/mol	Joback Method
hf	-140.74	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.600		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1780.40		NIST Webbook
rinpol	1780.40		NIST Webbook
tb	699.45	K	Joback Method
tc	919.33	K	Joback Method
tf	456.03	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.47	J/mol×K	699.45	Joback Method
cpg	629.21	J/mol×K	736.10	Joback Method
cpg	645.79	J/mol×K	772.74	Joback Method
cpg	661.26	J/mol×K	809.39	Joback Method
cpg	675.67	J/mol×K	846.04	Joback Method
cpg	689.03	J/mol×K	882.68	Joback Method
cpg	701.40	J/mol×K	919.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292534&Units=SI

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