Phenylacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H22O2/c1-14(2)10-11-17(12-15(3)4)20-18(19)13-16-8-6-5-7-9-16/h5-9,15,
InchiKey: KUQMVCQVSLJQDB-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
gf	256.38	kJ/mol	Joback Method
hf	-45.74	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	67.88	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.767		Crippen Method
mcvol	235.260	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1826.30		NIST Webbook
tb	718.89	K	Joback Method
tc	942.50	K	Joback Method
tf	451.58	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.70	J/mol×K	718.89	Joback Method
cpg	659.40	J/mol×K	756.16	Joback Method
cpg	675.92	J/mol×K	793.43	Joback Method
cpg	691.29	J/mol×K	830.69	Joback Method
cpg	705.57	J/mol×K	867.96	Joback Method
cpg	718.81	J/mol×K	905.23	Joback Method
cpg	731.06	J/mol×K	942.50	Joback Method

Sources

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=U292535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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