Phenylacetic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H24O2/c1-5-9-16(4)18(13-12-15(2)3)21-19(20)14-17-10-7-6-8-11-17/h6-8,

InchiKey: GATSJKTWXIWUMW-UHFFFAOYSA-N

Formula: C19H24O2

SMILES: C=C(C)C#CC(OC(=O)Cc1ccccc1)C(C)CCC

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	264.80	kJ/mol	Joback Method
hf	-66.38	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.157		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1904.00		NIST Webbook
tb	741.77	K	Joback Method
tc	961.86	K	Joback Method
tf	462.85	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.19	J/mol×K	741.77	Joback Method
cpg	715.11	J/mol×K	778.45	Joback Method
cpg	731.84	J/mol×K	815.13	Joback Method
cpg	747.41	J/mol×K	851.82	Joback Method
cpg	761.89	J/mol×K	888.50	Joback Method
cpg	775.33	J/mol×K	925.18	Joback Method
cpg	787.78	J/mol×K	961.86	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=U292536&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