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

Inchi: InChI=1S/C20H26O2/c1-5-9-17(4)19(14-12-16(2)3)22-20(21)15-13-18-10-7-6-8-11-18/h6

InchiKey: DUWKKLSTTBPJHA-UHFFFAOYSA-N

Formula: C20H26O2

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

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	273.22	kJ/mol	Joback Method
hf	-87.02	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.547		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2016.00		NIST Webbook
tb	764.65	K	Joback Method
tc	981.71	K	Joback Method
tf	474.12	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.76	J/mol×K	764.65	Joback Method
cpg	771.85	J/mol×K	800.83	Joback Method
cpg	788.73	J/mol×K	837.00	Joback Method
cpg	804.46	J/mol×K	873.18	Joback Method
cpg	819.10	J/mol×K	909.35	Joback Method
cpg	832.70	J/mol×K	945.53	Joback Method
cpg	845.30	J/mol×K	981.71	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=U299178&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