

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

Inchi:	InChI=1S/C19H24O2/c1-15(2)10-12-18(14-16(3)4)21-19(20)13-11-17-8-6-5-7-9-17/h5-9,
InchiKey:	NNQSPQLMDJEQMS-UHFFFAOYSA-N
Formula:	C19H24O2
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)CCc1ccccc1</chem>
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
mvol	249.350	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rmpol	1927.00		NIST Webbook
tb	741.77	K	Joback Method
tc	961.86	K	Joback Method
tf	462.85	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299177&Units=SI
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

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
mccvol:	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

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