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]: 284.40

Physical Properties

Property code	Value	Unit	Source
hfus	35.28	kJ/mol	Joback Method
hvap	87.58	kJ/mol	Cheméo Relay (1.0)
logp	4.157		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
rinpol	1904.00		NIST Webbook
tb	585.31	K	Cheméo Relay (1.0)

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292536&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature