Benzeneacetic acid, 1-methyl-2-propynyl ester

Other names: Phenylacetic acid, but-3-yn-2-yl ester
Inchi: InChI=1S/C12H12O2/c1-3-10(2)14-12(13)9-11-7-5-4-6-8-11/h1,4-8,10H,9H2,2H3
InchiKey: VXNDJPDQNAXPHL-UHFFFAOYSA-N
Formula: C12H12O2
SMILES: C#CC(C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 188.22
CAS: 54789-24-1

Physical Properties

Property code	Value	Unit	Source
gf	149.28	kJ/mol	Joback Method
hf	-12.66	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	53.21	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.794		Crippen Method
mcvol	155.020	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1369.80		NIST Webbook
tb	566.61	K	Joback Method
tc	791.92	K	Joback Method
tf	355.55	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.07	J/mol×K	566.61	Joback Method
cpg	369.34	J/mol×K	604.16	Joback Method
cpg	382.68	J/mol×K	641.71	Joback Method
cpg	395.13	J/mol×K	679.26	Joback Method
cpg	406.73	J/mol×K	716.81	Joback Method
cpg	417.51	J/mol×K	754.37	Joback Method
cpg	427.50	J/mol×K	791.92	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=C54789241&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