3-Phenylpropionic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C22H32O2/c1-2-3-4-5-6-7-8-9-10-11-15-20-24-22(23)19-18-21-16-13-12-14-17
InchiKey: VYQJQWHZRWGBSG-UHFFFAOYSA-N
Formula: C22H32O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	215.65	kJ/mol	Joback Method
hf	-233.38	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	78.15	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.697		Crippen Method
mcvol	295.920	ml/mol	McGowan Method
pc	1281.91	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	814.73	K	Joback Method
tc	1017.71	K	Joback Method
tf	542.38	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.02	J/mol×K	814.73	Joback Method
cpg	914.18	J/mol×K	848.56	Joback Method
cpg	931.20	J/mol×K	882.39	Joback Method
cpg	947.14	J/mol×K	916.22	Joback Method
cpg	962.03	J/mol×K	950.05	Joback Method
cpg	975.92	J/mol×K	983.88	Joback Method
cpg	988.86	J/mol×K	1017.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299180&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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