Butyric acid, 4-phenyl-, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C23H34O2/c1-2-3-4-5-6-7-8-9-10-11-15-21-25-23(24)20-16-19-22-17-13-12-14
InchiKey: PRODGKKCTFMQHQ-UHFFFAOYSA-N
Formula: C23H34O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCc1ccccc1
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	224.07	kJ/mol	Joback Method
hf	-254.02	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.087		Crippen Method
mcvol	310.010	ml/mol	McGowan Method
pc	1198.13	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	837.61	K	Joback Method
tc	1040.49	K	Joback Method
tf	553.65	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.92	J/mol×K	837.61	Joback Method
cpg	974.25	J/mol×K	871.42	Joback Method
cpg	991.42	J/mol×K	905.24	Joback Method
cpg	1007.49	J/mol×K	939.05	Joback Method
cpg	1022.49	J/mol×K	972.87	Joback Method
cpg	1036.48	J/mol×K	1006.68	Joback Method
cpg	1049.50	J/mol×K	1040.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406989&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
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