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

Inchi: InChI=1S/C23H34O2/c1-3-5-6-7-8-9-10-11-12-13-17-20-25-23(24)22(4-2)21-18-15-14-16
InchiKey: NIXUUFIWTOJRBJ-UHFFFAOYSA-N
Formula: C23H34O2
SMILES: CCCCCCCCCCC#CCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	221.63	kJ/mol	Joback Method
hf	-259.30	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	79.99	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.258		Crippen Method
mcvol	310.010	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	837.17	K	Joback Method
tc	1042.07	K	Joback Method
tf	538.65	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.41	J/mol×K	837.17	Joback Method
cpg	974.91	J/mol×K	871.32	Joback Method
cpg	992.22	J/mol×K	905.47	Joback Method
cpg	1008.39	J/mol×K	939.62	Joback Method
cpg	1023.46	J/mol×K	973.77	Joback Method
cpg	1037.49	J/mol×K	1007.92	Joback Method
cpg	1050.53	J/mol×K	1042.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406921&Units=SI

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