3-Cyclopentylpropionic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H36O2/c1-2-3-4-5-6-7-8-9-10-11-14-19-23-21(22)18-17-20-15-12-13-16-20

InchiKey: NCWPOQRAVJVACR-UHFFFAOYSA-N

Formula: C21H36O2

SMILES: CCCCCCCCCCC#CCOC(=O)CCC1CCCC1

Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	131.37	kJ/mol	Joback Method
hf	-388.79	kJ/mol	Joback Method
hfus	49.99	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.034		Crippen Method
mcvol	294.730	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	780.45	K	Joback Method
tc	975.87	K	Joback Method
tf	515.59	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.50	J/mol×K	780.45	Joback Method
cpg	936.88	J/mol×K	813.02	Joback Method
cpg	956.09	J/mol×K	845.59	Joback Method
cpg	974.17	J/mol×K	878.16	Joback Method
cpg	991.15	J/mol×K	910.73	Joback Method
cpg	1007.08	J/mol×K	943.30	Joback Method
cpg	1022.01	J/mol×K	975.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292471&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