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]: 320.52

Physical Properties

Property code	Value	Unit	Source
af	0.8098		Cheméo Relay (1.0)
gf	131.37	kJ/mol	Joback Method
hf	-510.66	kJ/mol	Cheméo Relay (1.0)
hfus	49.99	kJ/mol	Joback Method
hvap	103.29	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-6.69		Cheméo Relay (1.0)
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	621.12	K	Cheméo Relay (1.0)
tc	830.29	K	Cheméo Relay (1.0)
tf	269.34	K	Cheméo Relay (1.0)
vc	1.073	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292471&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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