3-Cyclopentylpropionic acid, dodec-9-ynyl ester

Other names: 3-cyclopentylpropionic acid, dodec-9-ynyl
Inchi: InChI=1S/C20H34O2/c1-2-3-4-5-6-7-8-9-10-13-18-22-20(21)17-16-19-14-11-12-15-19/h1
InchiKey: AVFPBHQFAAPMLJ-UHFFFAOYSA-N
Formula: C20H34O2
SMILES: CCC#CCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	122.95	kJ/mol	Joback Method
hf	-368.15	kJ/mol	Joback Method
hfus	47.40	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.644		Crippen Method
mcvol	280.640	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2299.20		NIST Webbook
rinpol	2299.20		NIST Webbook
tb	757.57	K	Joback Method
tc	953.57	K	Joback Method
tf	504.32	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.44	J/mol×K	757.57	Joback Method
cpg	876.68	J/mol×K	790.24	Joback Method
cpg	895.77	J/mol×K	822.90	Joback Method
cpg	913.75	J/mol×K	855.57	Joback Method
cpg	930.64	J/mol×K	888.24	Joback Method
cpg	946.50	J/mol×K	920.90	Joback Method
cpg	961.37	J/mol×K	953.57	Joback Method

Sources

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=U292272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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