Cyclobutanecarboxylic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-20-18(19)17-14-13-15-17/h17H,2-1

InchiKey: OYRRXIIIFQRANS-UHFFFAOYSA-N

Formula: C18H30O2

SMILES: CCCCCCCCCCC#CCOC(=O)C1CCC1

Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
gf	118.21	kJ/mol	Joback Method
hf	-320.71	kJ/mol	Joback Method
hfus	44.32	kJ/mol	Joback Method
hvap	67.06	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.864		Crippen Method
mcvol	252.460	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tb	707.54	K	Joback Method
tc	901.35	K	Joback Method
tf	485.30	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.83	J/mol×K	707.54	Joback Method
cpg	755.06	J/mol×K	739.84	Joback Method
cpg	773.27	J/mol×K	772.14	Joback Method
cpg	790.50	J/mol×K	804.44	Joback Method
cpg	806.77	J/mol×K	836.75	Joback Method
cpg	822.14	J/mol×K	869.05	Joback Method
cpg	836.63	J/mol×K	901.35	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=U299137&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