Cyclobutanecarboxylic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H22O2/c1-4-5-9-13(10-11(2)3)16-14(15)12-7-6-8-12/h11-13H,4,6-8,10H2,1

InchiKey: RVJZQJXADXKDGY-UHFFFAOYSA-N

Formula: C14H22O2

SMILES: CCC#CC(CC(C)C)OC(=O)C1CCC1

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	79.65	kJ/mol	Joback Method
hf	-248.71	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.158		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1460.00		NIST Webbook
tb	615.14	K	Joback Method
tc	826.07	K	Joback Method
tf	410.22	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.21	J/mol×K	615.14	Joback Method
cpg	535.91	J/mol×K	650.29	Joback Method
cpg	553.56	J/mol×K	685.45	Joback Method
cpg	570.19	J/mol×K	720.60	Joback Method
cpg	585.85	J/mol×K	755.76	Joback Method
cpg	600.56	J/mol×K	790.91	Joback Method
cpg	614.37	J/mol×K	826.07	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=U299133&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