Cyclobutanecarboxylic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C15H22O2/c1-11(2)8-9-14(10-12(3)4)17-15(16)13-6-5-7-13/h12-14H,1,5-7,10H

InchiKey: IOAICZNMDBXBSM-UHFFFAOYSA-N

Formula: C15H22O2

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

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	167.36	kJ/mol	Joback Method
hf	-153.71	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	59.01	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.324		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	634.58	K	Joback Method
tc	849.68	K	Joback Method
tf	405.77	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.51	J/mol×K	634.58	Joback Method
cpg	566.36	J/mol×K	670.43	Joback Method
cpg	584.09	J/mol×K	706.28	Joback Method
cpg	600.76	J/mol×K	742.13	Joback Method
cpg	616.40	J/mol×K	777.98	Joback Method
cpg	631.07	J/mol×K	813.83	Joback Method
cpg	644.81	J/mol×K	849.68	Joback Method

Sources

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=U299134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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