Cylobutanecarboxylic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C16H24O2/c1-5-7-13(4)15(11-10-12(2)3)18-16(17)14-8-6-9-14/h13-15H,2,5-9H

InchiKey: XUSFHBIEAJSZDC-UHFFFAOYSA-N

Formula: C16H24O2

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

Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	175.78	kJ/mol	Joback Method
hf	-174.35	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.714		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1604.00		NIST Webbook
tb	657.46	K	Joback Method
tc	869.10	K	Joback Method
tf	417.04	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.09	J/mol×K	657.46	Joback Method
cpg	620.27	J/mol×K	692.73	Joback Method
cpg	638.33	J/mol×K	728.01	Joback Method
cpg	655.31	J/mol×K	763.28	Joback Method
cpg	671.26	J/mol×K	798.55	Joback Method
cpg	686.23	J/mol×K	833.82	Joback Method
cpg	700.26	J/mol×K	869.10	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=U299135&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