(3Z),(2'E)-3-but-2'-enylidene-4,5,6,7-tetrahydrophth

Inchi: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h2-3,8H,4-7H2,1H3/b3-2+
InchiKey: UXDOUGRRBVGDEB-FWTOVJONSA-N
Formula: C12H14O2
SMILES: CC=CC=C1OC(=O)C2=C1CCCC2
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	78.45	kJ/mol	Joback Method
hf	-164.82	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.874		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	624.28	K	Joback Method
tc	865.17	K	Joback Method
tf	384.67	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.71	J/mol×K	624.28	Joback Method
cpg	407.78	J/mol×K	664.43	Joback Method
cpg	422.78	J/mol×K	704.58	Joback Method
cpg	436.76	J/mol×K	744.72	Joback Method
cpg	449.81	J/mol×K	784.87	Joback Method
cpg	461.99	J/mol×K	825.02	Joback Method
cpg	473.36	J/mol×K	865.17	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=R438218&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