Cyclopentanecarboxylic acid, 1-(2-butenyl)-2-oxo-, ethyl ester, (Z)-

Other names: Ethyl 1-[(2Z)-2-butenyl]-2-oxocyclopentanecarboxylate
cis-Cyclopentanecarboxylic acid, 1-(2-butenyl)-2-oxo-, ethyl ester
Inchi: InChI=1S/C12H18O3/c1-3-5-8-12(11(14)15-4-2)9-6-7-10(12)13/h3,5H,4,6-9H2,1-2H3/b5-
InchiKey: MUPFBGVUYDDKGG-HYXAFXHYSA-N
Formula: C12H18O3
SMILES: CC=CCC1(C(=O)OCC)CCCC1=O
Mol. weight [g/mol]: 210.27
CAS: 131534-41-3

Physical Properties

Property code	Value	Unit	Source
gf	-195.07	kJ/mol	Joback Method
hf	-480.57	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.255		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	637.75	K	Joback Method
tc	859.37	K	Joback Method
tf	395.10	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.25	J/mol×K	637.75	Joback Method
cpg	482.08	J/mol×K	674.69	Joback Method
cpg	498.06	J/mol×K	711.62	Joback Method
cpg	513.29	J/mol×K	748.56	Joback Method
cpg	527.87	J/mol×K	785.50	Joback Method
cpg	541.92	J/mol×K	822.43	Joback Method
cpg	555.52	J/mol×K	859.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131534413&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume