Methyl 4-(prop-1-en-2-yl)cyclohex-1-enecarboxylate

Other names: Methyl perillate
Inchi: InChI=1S/C11H16O2/c1-8(2)9-4-6-10(7-5-9)11(12)13-3/h6,9H,1,4-5,7H2,2-3H3
InchiKey: JMMLJZJUVKEVCK-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: C=C(C)C1CC=C(C(=O)OC)CC1
Mol. weight [g/mol]: 180.24
CAS: 26460-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-68.11	kJ/mol	Joback Method
hf	-298.90	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.462		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1394.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
tb	547.62	K	Joback Method
tc	761.02	K	Joback Method
tf	290.83	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.72	J/mol×K	547.62	Joback Method
cpg	382.53	J/mol×K	583.19	Joback Method
cpg	398.43	J/mol×K	618.75	Joback Method
cpg	413.43	J/mol×K	654.32	Joback Method
cpg	427.56	J/mol×K	689.89	Joback Method

cpg	440.83	J/mol×K	725.45	Joback Method
cpg	453.26	J/mol×K	761.02	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=C26460673&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