

2-(2-ethylcyclopropyl)-3-methyl-2-cyclopenten-1-one

Inchi:	InChI=1S/C11H16O/c1-3-8-6-9(8)11-7(2)4-5-10(11)12/h8-9H,3-6H2,1-2H3
InchiKey:	XXJJDRLPLQMPPO-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCC1CC1C=C(C)CCC1=O
Mol. weight [g/mol]:	164.24

Physical Properties

Property code	Value	Unit	Source
gf	27.15	kJ/mol	Joback Method
hf	-239.95	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	46.11	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.712		Crippen Method
mvol	141.400	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
ripol	1856.00		NIST Webbook
ripol	1851.00		NIST Webbook
tb	550.04	K	Joback Method
tc	772.71	K	Joback Method
tf	336.59	K	Joback Method
vc	0.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.34	J/mol×K	550.04	Joback Method
cpg	372.18	J/mol×K	587.15	Joback Method
cpg	389.05	J/mol×K	624.26	Joback Method
cpg	404.96	J/mol×K	661.38	Joback Method
cpg	419.96	J/mol×K	698.49	Joback Method
cpg	434.07	J/mol×K	735.60	Joback Method
cpg	447.32	J/mol×K	772.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R308291&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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