1,3-Cyclohexadiene-1-carboxylic acid, 2,6,6-trimethyl-, ethyl ester

Other names: Ethyl safranate
Ethyl 2,6,6-trimethyl-1,3-cyclohexadiene-1-carboxylate
Ethyle safranate
ethyl 2,6,6-trimethylcyclohexa-1,3-ene-1-carboxylate

Inchi: InChI=1S/C12H18O2/c1-5-14-11(13)10-9(2)7-6-8-12(10,3)4/h6-7H,5,8H2,1-4H3

InchiKey: KYEZYLFPHRVFBF-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: CCOC(=O)C1=C(C)C=CCC1(C)C

Mol. weight [g/mol]: 194.27

CAS: 35044-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-124.14	kJ/mol	Joback Method
hf	-373.63	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.852		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1981.00		NIST Webbook
tb	578.32	K	Joback Method
tc	791.31	K	Joback Method
tf	355.00	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	413.75	J/mol×K	578.32	Joback Method
cpg	429.91	J/mol×K	613.82	Joback Method
cpg	445.22	J/mol×K	649.32	Joback Method
cpg	459.76	J/mol×K	684.81	Joback Method
cpg	473.63	J/mol×K	720.31	Joback Method
cpg	486.91	J/mol×K	755.81	Joback Method
cpg	499.70	J/mol×K	791.31	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=C35044598&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume