

Ethyl (+)-camphorcarboxylate

Inchi:	InChI=1S/C13H20O3/c1-5-16-11(15)9-8-6-7-13(4,10(9)14)12(8,2)3/h8-9H,5-7H2,1-4H3
InchiKey:	ZYSAZWUGDXRNFJ-UHFFFAOYSA-N
Formula:	C13H20O3
SMILES:	CCOC(=O)C1C(=O)C2(C)CCC1C2(C)C
Mol. weight [g/mol]:	224.30
CAS:	22469-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-214.93	kJ/mol	Joback Method
hf	-564.91	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	55.01	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.191		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	649.84	K	Joback Method
tc	874.31	K	Joback Method
tf	448.33	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.93	J/molxK	649.84	Joback Method
cpg	541.29	J/molxK	687.25	Joback Method
cpg	558.90	J/molxK	724.66	Joback Method
cpg	575.97	J/molxK	762.08	Joback Method
cpg	592.72	J/molxK	799.49	Joback Method
cpg	609.37	J/molxK	836.90	Joback Method
cpg	626.11	J/molxK	874.31	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=C22469701&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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