2-ethyl isomenthone

Inchi: InChI=1S/C12H22O/c1-5-10-9(4)6-7-11(8(2)3)12(10)13/h8-11H,5-7H2,1-4H3/t9-,10?,11-,
InchiKey: VXGVKPGULBZBOZ-GLYLRITDSA-N
Formula: C12H22O
SMILES: CCC1C(=O)C(C(C)C)CCC1C
Mol. weight [g/mol]: 182.30

Physical Properties

Property code	Value	Unit	Source
gf	-65.84	kJ/mol	Joback Method
hf	-420.35	kJ/mol	Joback Method
hfus	16.80	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.284		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1294.00		NIST Webbook
tb	551.55	K	Joback Method
tc	762.55	K	Joback Method
tf	277.12	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.61	J/mol×K	551.55	Joback Method
cpg	460.22	J/mol×K	586.72	Joback Method
cpg	480.83	J/mol×K	621.88	Joback Method
cpg	500.42	J/mol×K	657.05	Joback Method
cpg	518.98	J/mol×K	692.22	Joback Method
cpg	536.51	J/mol×K	727.39	Joback Method
cpg	552.99	J/mol×K	762.55	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=R411253&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