«alpha»-Isofenchyl acetate

Inchi: InChI=1S/C12H20O2/c1-8(13)14-10-11(2,3)9-5-6-12(10,4)7-9/h9-10H,5-7H2,1-4H3/t9-,1
InchiKey: JUWUWIGZUVEFQB-FOGDFJRCSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1C2(C)CCC(C2)C1(C)C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-406.57	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1236.00		NIST Webbook
tb	559.14	K	Joback Method
tc	774.82	K	Joback Method
tf	368.84	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.90	J/mol×K	559.14	Joback Method
cpg	456.54	J/mol×K	595.09	Joback Method
cpg	474.00	J/mol×K	631.03	Joback Method
cpg	490.47	J/mol×K	666.98	Joback Method
cpg	506.18	J/mol×K	702.93	Joback Method
cpg	521.34	J/mol×K	738.88	Joback Method
cpg	536.18	J/mol×K	774.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R410369&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume