«alpha»-Isoamylionone

Inchi: InChI=1S/C18H30O/c1-14(2)8-6-10-16(19)11-12-17-15(3)9-7-13-18(17,4)5/h11-12,14H,6
InchiKey: RNFIPQAOLNYJEF-VAWYXSNFSA-N
Formula: C18H30O
SMILES: CC1=C(C=CC(=O)CCCC(C)C)C(C)(C)CCC1
Mol. weight [g/mol]: 262.43

Physical Properties

Property code	Value	Unit	Source
gf	79.20	kJ/mol	Joback Method
hf	-311.09	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.465		Crippen Method
mcvol	246.590	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	1954.00		NIST Webbook
tb	697.74	K	Joback Method
tc	904.12	K	Joback Method
tf	379.55	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.13	J/mol×K	697.74	Joback Method
cpg	725.45	J/mol×K	732.14	Joback Method
cpg	744.86	J/mol×K	766.53	Joback Method
cpg	763.48	J/mol×K	800.93	Joback Method
cpg	781.43	J/mol×K	835.33	Joback Method
cpg	798.84	J/mol×K	869.72	Joback Method
cpg	815.82	J/mol×K	904.12	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=R572219&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