cis-Valerenyl isovalerate

Inchi: InChI=1S/C20H32O2/c1-13(2)10-19(21)22-12-14(3)11-17-8-6-15(4)18-9-7-16(5)20(17)18
InchiKey: QFANMAOKAWEBQA-SDNWHVSQSA-N
Formula: C20H32O2
SMILES: CC(=CC1CCC(C)C2CCC(C)=C12)COC(=O)CC(C)C
Mol. weight [g/mol]: 304.47
CAS: 101527-75-7

Physical Properties

Property code	Value	Unit	Source
gf	41.02	kJ/mol	Joback Method
hf	-457.16	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	70.57	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.295		Crippen Method
mcvol	269.780	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2058.40		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	2058.40		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	767.63	K	Joback Method
tc	975.63	K	Joback Method
tf	400.16	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.66	J/mol×K	767.63	Joback Method
cpg	865.58	J/mol×K	802.30	Joback Method
cpg	885.23	J/mol×K	836.96	Joback Method
cpg	903.67	J/mol×K	871.63	Joback Method
cpg	920.96	J/mol×K	906.29	Joback Method

cpg	937.17	J/mol×K	940.96	Joback Method
cpg	952.35	J/mol×K	975.63	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=C101527757&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume