cis-Valerenyl acetate

Inchi: InChI=1S/C17H26O2/c1-11(10-19-14(4)18)9-15-7-5-12(2)16-8-6-13(3)17(15)16/h9,12,15
InchiKey: GMTBKCJRMNJNFL-LUAWRHEFSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CC1CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]: 262.39
CAS: 101527-78-0

Physical Properties

Property code	Value	Unit	Source
gf	18.20	kJ/mol	Joback Method
hf	-389.96	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	64.28	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1828.60		NIST Webbook
rinpol	1804.60		NIST Webbook
rinpol	1804.60		NIST Webbook
tb	699.43	K	Joback Method
tc	911.60	K	Joback Method
tf	381.35	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.84	J/mol×K	699.43	Joback Method
cpg	690.13	J/mol×K	734.79	Joback Method
cpg	709.20	J/mol×K	770.15	Joback Method
cpg	727.09	J/mol×K	805.51	Joback Method
cpg	743.88	J/mol×K	840.88	Joback Method
cpg	759.60	J/mol×K	876.24	Joback Method

cpg	774.33	J/mol×K	911.60	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=C101527780&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