trans-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-PODTTWMBSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC(C)=CC1CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
hfus	32.95	kJ/mol	Joback Method
logp	4.268		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
rinpol	1785.00		NIST Webbook
rinpol	1796.00		NIST Webbook
ripol	2224.00		NIST Webbook
ripol	2224.00		NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225017&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices