pentacosyl acetate

Inchi: InChI=1S/C27H54O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: XTQVKPPRJQPCIJ-UHFFFAOYSA-N
Formula: C27H54O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 410.72

Physical Properties

Property code	Value	Unit	Source
gf	-57.46	kJ/mol	Joback Method
hf	-845.41	kJ/mol	Joback Method
hfus	68.47	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-9.99		Crippen Method
logp	9.542		Crippen Method
mcvol	398.730	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	2895.22		NIST Webbook
rinpol	2895.22		NIST Webbook
tb	893.45	K	Joback Method
tc	1097.77	K	Joback Method
tf	466.21	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.54	J/mol×K	893.45	Joback Method
cpg	1374.21	J/mol×K	927.50	Joback Method
cpg	1396.42	J/mol×K	961.56	Joback Method
cpg	1417.22	J/mol×K	995.61	Joback Method
cpg	1436.68	J/mol×K	1029.66	Joback Method
cpg	1454.85	J/mol×K	1063.71	Joback Method
cpg	1471.80	J/mol×K	1097.77	Joback Method
dvisc	0.0007281	Pa×s	466.21	Joback Method

dvisc	0.0002915	Pa×s	537.42	Joback Method
dvisc	0.0001446	Pa×s	608.62	Joback Method
dvisc	0.0000831	Pa×s	679.83	Joback Method
dvisc	0.0000530	Pa×s	751.04	Joback Method
dvisc	0.0000366	Pa×s	822.24	Joback Method
dvisc	0.0000268	Pa×s	893.45	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=R437988&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
dvisc:	Dynamic viscosity
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