2,13-Diacetoxyheptadecane

Inchi: InChI=1S/C21H40O4/c1-5-6-16-21(25-20(4)23)17-14-12-10-8-7-9-11-13-15-18(2)24-19(3
InchiKey: YIWUNSWAUYLXPP-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCC(CCCCCCCCCCC(C)OC(C)=O)OC(C)=O
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-976.93	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.961		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	2279.00		NIST Webbook
tb	831.58	K	Joback Method
tc	1019.89	K	Joback Method
tf	440.75	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.20	J/mol×K	831.58	Joback Method
cpg	1049.98	J/mol×K	862.97	Joback Method
cpg	1067.62	J/mol×K	894.35	Joback Method
cpg	1084.13	J/mol×K	925.74	Joback Method
cpg	1099.54	J/mol×K	957.12	Joback Method
cpg	1113.87	J/mol×K	988.51	Joback Method
cpg	1127.14	J/mol×K	1019.89	Joback Method
dvisc	0.0010562	Pa×s	440.75	Joback Method
dvisc	0.0004270	Pa×s	505.89	Joback Method

dvisc	0.0002123	Pa×s	571.03	Joback Method
dvisc	0.0001217	Pa×s	636.16	Joback Method
dvisc	0.0000774	Pa×s	701.30	Joback Method
dvisc	0.0000532	Pa×s	766.44	Joback Method
dvisc	0.0000387	Pa×s	831.58	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=R413477&Units=SI

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