Dimethyl 3,6,9,12,15,18,21,24,27-nonaoxanonacosane-1,29-

Inchi: InChI=1S/C22H42O13/c1-25-21(23)19-34-17-15-32-13-11-30-9-7-28-5-3-27-4-6-29-8-10

InchiKey: NYAFCYGDUIRDMW-UHFFFAOYSA-N

Formula: C22H42O13

SMILES: COC(=O)COCCOCCOCCOCCOCCOCCOCCOCCOCC(=O)OC

Mol. weight [g/mol]: 514.56

Physical Properties

Property code	Value	Unit	Source
gf	-1278.48	kJ/mol	Joback Method
hf	-2176.99	kJ/mol	Joback Method
hfus	69.00	kJ/mol	Joback Method
hvap	104.57	kJ/mol	Joback Method
log10ws	1.46		Crippen Method
logp	-0.518		Crippen Method
mcvol	388.550	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	3436.20		NIST Webbook
rinpol	3436.20		NIST Webbook
tb	1057.12	K	Joback Method
tc	1329.23	K	Joback Method
tf	682.09	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.45	J/mol×K	1057.12	Joback Method
cpg	1365.96	J/mol×K	1102.47	Joback Method
cpg	1371.78	J/mol×K	1147.82	Joback Method
cpg	1372.71	J/mol×K	1193.18	Joback Method
cpg	1368.53	J/mol×K	1238.53	Joback Method
cpg	1359.05	J/mol×K	1283.88	Joback Method
cpg	1344.05	J/mol×K	1329.23	Joback Method
dvisc	0.0000216	Pa×s	682.09	Joback Method

dvisc	0.0000129	Pa×s	744.60	Joback Method
dvisc	0.0000083	Pa×s	807.10	Joback Method
dvisc	0.0000057	Pa×s	869.61	Joback Method
dvisc	0.0000041	Pa×s	932.11	Joback Method
dvisc	0.0000031	Pa×s	994.61	Joback Method
dvisc	0.0000024	Pa×s	1057.12	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=R578099&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