Butyl 2,5,8,11,14,17,20,23,26,29,32-undecaoxatetratriacc

Inchi: InChI=1S/C27H54O13/c1-3-4-5-40-27(28)26-39-25-24-38-23-22-37-21-20-36-19-18-35-1

InchiKey: MAVPKUMTKBZCCY-UHFFFAOYSA-N

Formula: C27H54O13

SMILES: CCCCOC(=O)COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOC

Mol. weight [g/mol]: 586.71

Physical Properties

Property code	Value	Unit	Source
gf	-1212.46	kJ/mol	Joback Method
hf	-2299.83	kJ/mol	Joback Method
hfus	81.54	kJ/mol	Joback Method
hvap	111.36	kJ/mol	Joback Method
log10ws	0.05		Crippen Method
logp	1.142		Crippen Method
mcvol	463.300	ml/mol	McGowan Method
pc	640.60	kPa	Joback Method
rinpol	3832.10		NIST Webbook
rinpol	3832.10		NIST Webbook
tb	1140.07	K	Joback Method
tc	1500.62	K	Joback Method
tf	710.74	K	Joback Method
vc	1.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1672.92	J/mol×K	1140.07	Joback Method
cpg	1597.88	J/mol×K	1440.53	Joback Method
cpg	1634.65	J/mol×K	1380.44	Joback Method
cpg	1660.07	J/mol×K	1320.34	Joback Method
cpg	1674.61	J/mol×K	1260.25	Joback Method
cpg	1678.74	J/mol×K	1200.16	Joback Method
cpg	1549.30	J/mol×K	1500.62	Joback Method
dvisc	0.0000008	Pa×s	1140.07	Joback Method

dvisc	0.0000011	Pa×s	1068.52	Joback Method
dvisc	0.0000014	Pa×s	996.96	Joback Method
dvisc	0.0000021	Pa×s	925.41	Joback Method
dvisc	0.0000031	Pa×s	853.85	Joback Method
dvisc	0.0000051	Pa×s	782.30	Joback Method
dvisc	0.0000091	Pa×s	710.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R578113&Units=SI
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

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