1-Methyl-2-methoxyethyl behenoate

Inchi: InChI=1S/C26H52O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26(27
InchiKey: OLPWCQVTDGVJNQ-UHFFFAOYSA-N
Formula: C26H52O3
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 412.69

Physical Properties

Property code	Value	Unit	Source
gf	-173.32	kJ/mol	Joback Method
hf	-962.27	kJ/mol	Joback Method
hfus	63.55	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.386		Crippen Method
mcvol	390.510	ml/mol	McGowan Method
pc	739.63	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	892.55	K	Joback Method
tc	1095.41	K	Joback Method
tf	462.17	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.14	J/mol×K	892.55	Joback Method
cpg	1419.23	J/mol×K	1061.60	Joback Method
cpg	1402.24	J/mol×K	1027.79	Joback Method
cpg	1383.88	J/mol×K	993.98	Joback Method
cpg	1364.10	J/mol×K	960.17	Joback Method
cpg	1342.87	J/mol×K	926.36	Joback Method
cpg	1434.88	J/mol×K	1095.41	Joback Method
dvisc	0.0000211	Pa×s	892.55	Joback Method

dvisc	0.0000291	Pa×s	820.82	Joback Method
dvisc	0.0000426	Pa×s	749.09	Joback Method
dvisc	0.0000679	Pa×s	677.36	Joback Method
dvisc	0.0001206	Pa×s	605.63	Joback Method
dvisc	0.0002500	Pa×s	533.90	Joback Method
dvisc	0.0006499	Pa×s	462.17	Joback Method

Sources

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=R540064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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