1-Methyl-2-methoxyethyl stearate

Inchi: InChI=1S/C22H44O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(23)25-21(2)20-2
InchiKey: FSAWRPXLQQIUGA-UHFFFAOYSA-N
Formula: C22H44O3
SMILES: CCCCCCCCCCCCCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 356.58

Physical Properties

Property code	Value	Unit	Source
gf	-207.00	kJ/mol	Joback Method
hf	-879.71	kJ/mol	Joback Method
hfus	53.19	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.826		Crippen Method
mcvol	334.150	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	2392.00		NIST Webbook
tb	801.03	K	Joback Method
tc	981.83	K	Joback Method
tf	417.09	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.16	J/mol×K	801.03	Joback Method
cpg	1156.97	J/mol×K	951.70	Joback Method
cpg	1140.73	J/mol×K	921.57	Joback Method
cpg	1123.45	J/mol×K	891.43	Joback Method
cpg	1105.11	J/mol×K	861.30	Joback Method
cpg	1085.69	J/mol×K	831.16	Joback Method
cpg	1172.19	J/mol×K	981.83	Joback Method
dvisc	0.0000384	Pa×s	801.03	Joback Method
dvisc	0.0000526	Pa×s	737.04	Joback Method

dvisc	0.0000766	Pa×s	673.05	Joback Method
dvisc	0.0001207	Pa×s	609.06	Joback Method
dvisc	0.0002115	Pa×s	545.07	Joback Method
dvisc	0.0004302	Pa×s	481.08	Joback Method
dvisc	0.0010883	Pa×s	417.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540222&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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