2-Methoxyethyl stearate

Inchi: InChI=1S/C21H42O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(22)24-20-19-23-2
InchiKey: WWFMRRQOYPKLIM-UHFFFAOYSA-N
Formula: C21H42O3
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 342.56
CAS: 111-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-212.98	kJ/mol	Joback Method
hf	-853.79	kJ/mol	Joback Method
hfus	54.12	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.438		Crippen Method
mcvol	320.060	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	2374.00		NIST Webbook
tb	778.59	K	Joback Method
tc	955.33	K	Joback Method
tf	420.82	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.70	J/mol×K	778.59	Joback Method
cpg	1022.68	J/mol×K	808.05	Joback Method
cpg	1041.64	J/mol×K	837.50	Joback Method
cpg	1059.60	J/mol×K	866.96	Joback Method
cpg	1076.58	J/mol×K	896.41	Joback Method
cpg	1092.59	J/mol×K	925.87	Joback Method
cpg	1107.66	J/mol×K	955.33	Joback Method
dvisc	0.0010020	Pa×s	420.82	Joback Method

dvisc	0.0004416	Pa×s	480.45	Joback Method
dvisc	0.0002332	Pa×s	540.08	Joback Method
dvisc	0.0001398	Pa×s	599.70	Joback Method
dvisc	0.0000920	Pa×s	659.33	Joback Method
dvisc	0.0000649	Pa×s	718.96	Joback Method
dvisc	0.0000482	Pa×s	778.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111091&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