heptadecanoic acid, 2-methoxyethyl ester

Other names: 2-methoxyethyl heptadecanoate
Inchi: InChI=1S/C20H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(21)23-19-18-22-2/h3
InchiKey: FJMOQEMYOPDDEY-UHFFFAOYSA-N
Formula: C20H40O3
SMILES: CCCCCCCCCCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 328.53

Physical Properties

Property code	Value	Unit	Source
gf	-221.40	kJ/mol	Joback Method
hf	-833.15	kJ/mol	Joback Method
hfus	51.53	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	6.047		Crippen Method
mcvol	305.970	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	755.71	K	Joback Method
tc	929.49	K	Joback Method
tf	409.55	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.52	J/mol×K	755.71	Joback Method
cpg	961.02	J/mol×K	784.67	Joback Method
cpg	979.57	J/mol×K	813.64	Joback Method
cpg	997.19	J/mol×K	842.60	Joback Method
cpg	1013.87	J/mol×K	871.56	Joback Method
cpg	1029.66	J/mol×K	900.53	Joback Method
cpg	1044.55	J/mol×K	929.49	Joback Method

dvisc	0.0011174	Pa×s	409.55	Joback Method
dvisc	0.0004975	Pa×s	467.24	Joback Method
dvisc	0.0002646	Pa×s	524.94	Joback Method
dvisc	0.0001595	Pa×s	582.63	Joback Method
dvisc	0.0001053	Pa×s	640.32	Joback Method
dvisc	0.0000745	Pa×s	698.02	Joback Method
dvisc	0.0000555	Pa×s	755.71	Joback Method

Sources

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=U398008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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