

1-Methyl-2-methoxyethyl palmitate

Inchi:	InChI=1S/C20H40O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(21)23-19(2)18-22-3/h
InchiKey:	QBFQJGFRZZJVBR-UHFFFAOYSA-N
Formula:	C20H40O3
SMILES:	CCCCCCCCCCCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]:	328.53

Physical Properties

Property code	Value	Unit	Source
gf	-223.84	kJ/mol	Joback Method
hf	-838.43	kJ/mol	Joback Method
hfus	48.01	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	6.046		Crippen Method
mcvol	305.970	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
rinpol	2194.00		NIST Webbook
tb	755.27	K	Joback Method
tc	930.04	K	Joback Method
tf	394.55	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.96	J/molxK	755.27	Joback Method
cpg	1030.55	J/molxK	900.91	Joback Method
cpg	1014.71	J/molxK	871.78	Joback Method
cpg	997.95	J/molxK	842.65	Joback Method
cpg	980.25	J/molxK	813.53	Joback Method
cpg	961.59	J/molxK	784.40	Joback Method
cpg	1045.47	J/molxK	930.04	Joback Method
dvisc	0.0000512	Paxs	755.27	Joback Method
dvisc	0.0000699	Paxs	695.15	Joback Method

dvisc	0.0001012	Paxs	635.03	Joback Method
dvisc	0.0001585	Paxs	574.91	Joback Method
dvisc	0.0002755	Paxs	514.79	Joback Method
dvisc	0.0005542	Paxs	454.67	Joback Method
dvisc	0.0013798	Paxs	394.55	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=R540193&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

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