3-Methoxybutyl pentadecanoate

Inchi: InChI=1S/C20H40O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20(21)23-18-17-19(2)22-3/h1
InchiKey: AXCJHRVOWOZDEQ-UHFFFAOYSA-N
Formula: C20H40O3
SMILES: CCCCCCCCCCCCCCC(=O)OCCC(C)OC
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	2222.00		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/mol×K	755.27	Joback Method
cpg	1030.55	J/mol×K	900.91	Joback Method
cpg	1014.71	J/mol×K	871.78	Joback Method
cpg	997.95	J/mol×K	842.65	Joback Method
cpg	980.25	J/mol×K	813.53	Joback Method
cpg	961.59	J/mol×K	784.40	Joback Method
cpg	1045.47	J/mol×K	930.04	Joback Method
dvisc	0.0000512	Pa×s	755.27	Joback Method
dvisc	0.0000699	Pa×s	695.15	Joback Method

dvisc	0.0001012	Pa×s	635.03	Joback Method
dvisc	0.0001585	Pa×s	574.91	Joback Method
dvisc	0.0002755	Pa×s	514.79	Joback Method
dvisc	0.0005542	Pa×s	454.67	Joback Method
dvisc	0.0013798	Pa×s	394.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541012&Units=SI

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