

3-Methoxybutyl nonadecanoate

Inchi:	InChI=1S/C24H48O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24(25)27-22-21
InchiKey:	GEKFNXPKIHVGBV-UHFFFAOYSA-N
Formula:	C24H48O3
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	384.64

Physical Properties

Property code	Value	Unit	Source
gf	-190.16	kJ/mol	Joback Method
hf	-920.99	kJ/mol	Joback Method
hfus	58.37	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.606		Crippen Method
mcvol	362.330	ml/mol	McGowan Method
pc	823.37	kPa	Joback Method
rinsol	2603.00		NIST Webbook
tb	846.79	K	Joback Method
tc	1036.77	K	Joback Method
tf	439.63	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.40	J/molxK	846.79	Joback Method
cpg	1212.95	J/molxK	878.45	Joback Method
cpg	1233.21	J/molxK	910.12	Joback Method
cpg	1252.24	J/molxK	941.78	Joback Method
cpg	1270.05	J/molxK	973.44	Joback Method
cpg	1286.67	J/molxK	1005.11	Joback Method
cpg	1302.14	J/molxK	1036.77	Joback Method
dvisc	0.0008462	Paxs	439.63	Joback Method
dvisc	0.0003297	Paxs	507.49	Joback Method

dvisc	0.0001605	Paxs	575.35	Joback Method
dvisc	0.0000909	Paxs	643.21	Joback Method
dvisc	0.0000574	Paxs	711.07	Joback Method
dvisc	0.0000393	Paxs	778.93	Joback Method
dvisc	0.0000286	Paxs	846.79	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=R540980&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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