

3-Methoxybutyl tridecanoate

Inchi:	InChI=1S/C18H36O3/c1-4-5-6-7-8-9-10-11-12-13-14-18(19)21-16-15-17(2)20-3/h17H,4-
InchiKey:	TYILNKNHKJQXQP-UHFFFAOYSA-N
Formula:	C18H36O3
SMILES:	CCCCCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	300.48

Physical Properties

Property code	Value	Unit	Source
gf	-240.68	kJ/mol	Joback Method
hf	-797.15	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	5.266		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpola	2023.00		NIST Webbook
rinpola	2023.00		NIST Webbook
tb	709.51	K	Joback Method
tc	880.87	K	Joback Method
tf	372.01	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.40	J/molxK	709.51	Joback Method
cpg	841.19	J/molxK	738.07	Joback Method
cpg	859.11	J/molxK	766.63	Joback Method
cpg	876.18	J/molxK	795.19	Joback Method
cpg	892.40	J/molxK	823.75	Joback Method
cpg	907.79	J/molxK	852.31	Joback Method
cpg	922.36	J/molxK	880.87	Joback Method
dvisc	0.0017203	Paxs	372.01	Joback Method

dvisc	0.0007033	Paxs	428.26	Joback Method
dvisc	0.0003539	Paxs	484.51	Joback Method
dvisc	0.0002054	Paxs	540.76	Joback Method
dvisc	0.0001321	Paxs	597.01	Joback Method
dvisc	0.0000917	Paxs	653.26	Joback Method
dvisc	0.0000674	Paxs	709.51	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=R541052&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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