Dodecanoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C18H36O3/c1-4-5-6-7-8-9-10-11-12-13-18(19)21-16-17(2)14-15-20-3/h17H,4-1

InchiKey: ZGVULAWWXXRQCZ-UHFFFAOYSA-N

Formula: C18H36O3

SMILES: CCCCCCCCCCCC(=O)OCC(C)CCOC

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	-5.07		Crippen Method
logp	5.123		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	709.51	K	Joback Method
tc	880.87	K	Joback Method
tf	372.01	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.40	J/mol×K	709.51	Joback Method
cpg	841.19	J/mol×K	738.07	Joback Method
cpg	859.11	J/mol×K	766.63	Joback Method
cpg	876.18	J/mol×K	795.19	Joback Method
cpg	892.40	J/mol×K	823.75	Joback Method
cpg	907.79	J/mol×K	852.31	Joback Method
cpg	922.36	J/mol×K	880.87	Joback Method
dvisc	0.0017203	Pa×s	372.01	Joback Method
dvisc	0.0007033	Pa×s	428.26	Joback Method

dvisc	0.0003539	Pa×s	484.51	Joback Method
dvisc	0.0002054	Pa×s	540.76	Joback Method
dvisc	0.0001321	Pa×s	597.01	Joback Method
dvisc	0.0000917	Pa×s	653.26	Joback Method
dvisc	0.0000674	Pa×s	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=U360544&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