Dodecanoic acid tert-butyl ester

Other names: Dodecanoic acid, 1,1-dimethylethyl ester
Lauric acid, tert-butyl ester
Inchi: InChI=1S/C16H32O2/c1-5-6-7-8-9-10-11-12-13-14-15(17)18-16(2,3)4/h5-14H2,1-4H3
InchiKey: WJXKWIFHRZWPET-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCCCCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 256.42
CAS: 7143-18-2

Physical Properties

Property code	Value	Unit	Source
chl	-10052.00 ± 12.00	kJ/mol	NIST Webbook
gf	-147.24	kJ/mol	Joback Method
hf	-627.12	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	59.07	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.249		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1382.99	kPa	Joback Method
tb	638.54	K	Joback Method
tc	812.42	K	Joback Method
tf	344.66	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.28	J/mol×K	638.54	Joback Method
cpg	696.75	J/mol×K	667.52	Joback Method
cpg	714.36	J/mol×K	696.50	Joback Method
cpg	731.14	J/mol×K	725.48	Joback Method
cpg	747.10	J/mol×K	754.46	Joback Method
cpg	762.29	J/mol×K	783.44	Joback Method

cpg	776.72	J/mol×K	812.42	Joback Method
dvisc	0.0027072	Pa×s	344.66	Joback Method
dvisc	0.0011277	Pa×s	393.64	Joback Method
dvisc	0.0005702	Pa×s	442.62	Joback Method
dvisc	0.0003303	Pa×s	491.60	Joback Method
dvisc	0.0002112	Pa×s	540.58	Joback Method
dvisc	0.0001455	Pa×s	589.56	Joback Method
dvisc	0.0001061	Pa×s	638.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7143182&Units=SI
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

Legend

chl: Standard liquid enthalpy of combustion
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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