Octanoic acid-tert butyl ester

Other names: Octanoic acid, 1,1-dimethylethyl ester
Octanoic acid, t-butyl ester
tert-butyl octanoate
Inchi: InChI=1S/C12H24O2/c1-5-6-7-8-9-10-11(13)14-12(2,3)4/h5-10H2,1-4H3
InchiKey: BRHAUGJKIFZHDU-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 200.32
CAS: 5457-66-9

Physical Properties

Property code	Value	Unit	Source
chl	-7453.00 ± 13.00	kJ/mol	NIST Webbook
gf	-180.92	kJ/mol	Joback Method
hf	-544.56	kJ/mol	Joback Method
hfus	22.21	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.689		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
tb	547.02	K	Joback Method
tc	725.77	K	Joback Method
tf	299.58	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.06	J/mol×K	547.02	Joback Method
cpg	483.65	J/mol×K	576.81	Joback Method
cpg	499.47	J/mol×K	606.60	Joback Method
cpg	514.55	J/mol×K	636.40	Joback Method
cpg	528.91	J/mol×K	666.19	Joback Method

cpg	542.58	J/mol×K	695.98	Joback Method
cpg	555.57	J/mol×K	725.77	Joback Method
dvisc	0.0038453	Pa×s	299.58	Joback Method
dvisc	0.0016806	Pa×s	340.82	Joback Method
dvisc	0.0008783	Pa×s	382.06	Joback Method
dvisc	0.0005208	Pa×s	423.30	Joback Method
dvisc	0.0003389	Pa×s	464.54	Joback Method
dvisc	0.0002365	Pa×s	505.78	Joback Method
dvisc	0.0001743	Pa×s	547.02	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=C5457669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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