

1-tert-Butoxypropan-2-yl nonanoate

Inchi:	InChI=1S/C16H32O3/c1-6-7-8-9-10-11-12-15(17)19-14(2)13-18-16(3,4)5/h14H,6-13H2,1
InchiKey:	FGLVSVRSIWAKB-UHFFFAOYSA-N
Formula:	C16H32O3
SMILES:	CCCCCCCCC(=O)OC(C)COC(C)(C)C
Mol. weight [g/mol]:	272.42

Physical Properties

Property code	Value	Unit	Source
gf	-254.68	kJ/mol	Joback Method
hf	-764.62	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	61.09	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.484		Crippen Method
mvol	249.610	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	1669.00		NIST Webbook
tb	660.52	K	Joback Method
tc	836.93	K	Joback Method
tf	351.89	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.45	J/molxK	660.52	Joback Method
cpg	793.07	J/molxK	807.53	Joback Method
cpg	778.02	J/molxK	778.13	Joback Method
cpg	762.16	J/molxK	748.73	Joback Method
cpg	745.45	J/molxK	719.32	Joback Method
cpg	727.89	J/molxK	689.92	Joback Method
cpg	807.32	J/molxK	836.93	Joback Method
dvisc	0.0000752	Paxs	660.52	Joback Method
dvisc	0.0001047	Paxs	609.08	Joback Method

dvisc	0.0001549	Paxs	557.64	Joback Method
dvisc	0.0002481	Paxs	506.20	Joback Method
dvisc	0.0004422	Paxs	454.77	Joback Method
dvisc	0.0009131	Paxs	403.33	Joback Method
dvisc	0.0023309	Paxs	351.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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