

2-nonyl octanoate

Inchi: InChI=1S/C17H34O2/c1-4-6-8-10-12-14-16(3)19-17(18)15-13-11-9-7-5-2/h16H,4-15H2,1-3H
InchiKey: OHAICYQKNMRREW-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCCCCCC(=O)OC(C)CCCCCCC
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	-144.10	kJ/mol	Joback Method
hf	-644.29	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.639		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
ripol	1982.00		NIST Webbook
ripol	1982.00		NIST Webbook
tb	664.21	K	Joback Method
tc	833.82	K	Joback Method
tf	338.51	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.67	J/mol×K	664.21	Joback Method
cpg	751.27	J/mol×K	692.48	Joback Method
cpg	769.05	J/mol×K	720.75	Joback Method
cpg	786.03	J/mol×K	749.02	Joback Method
cpg	802.22	J/mol×K	777.28	Joback Method
cpg	817.65	J/mol×K	805.55	Joback Method
cpg	832.34	J/mol×K	833.82	Joback Method
dvisc	0.0028787	Pa×s	338.51	Joback Method

dvisc	0.0011177	Pa×s	392.79	Joback Method
dvisc	0.0005461	Pa×s	447.08	Joback Method
dvisc	0.0003116	Pa×s	501.36	Joback Method
dvisc	0.0001983	Pa×s	555.64	Joback Method
dvisc	0.0001368	Pa×s	609.93	Joback Method
dvisc	0.0001003	Pa×s	664.21	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=R519703&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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