

Adipic acid, nonyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C20H36O4/c1-4-6-7-8-9-10-13-17-23-19(21)15-11-12-16-20(22)24-18(3)14-5-2
InchiKey:	XMPZZUIJHYGPKU-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	<chem>C=CCC(C)OC(=O)CCCC(=O)OCCCCCCCCC</chem>
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-264.92	kJ/mol	Joback Method
hf	-825.58	kJ/mol	Joback Method
hfus	48.33	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2247.00		NIST Webbook
tb	805.82	K	Joback Method
tc	990.69	K	Joback Method
tf	442.72	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.73	J/molxK	805.82	Joback Method
cpg	960.52	J/molxK	836.63	Joback Method
cpg	977.28	J/molxK	867.44	Joback Method
cpg	993.04	J/molxK	898.25	Joback Method
cpg	1007.82	J/molxK	929.06	Joback Method
cpg	1021.64	J/molxK	959.88	Joback Method
cpg	1034.51	J/molxK	990.69	Joback Method
dvisc	0.0010021	Paxs	442.72	Joback Method
dvisc	0.0004555	Paxs	503.24	Joback Method

dvisc	0.0002452	Paxs	563.75	Joback Method
dvisc	0.0001489	Paxs	624.27	Joback Method
dvisc	0.0000987	Paxs	684.79	Joback Method
dvisc	0.0000700	Paxs	745.30	Joback Method
dvisc	0.0000522	Paxs	805.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U354125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/28-258-5/Adipic-acid-nonyl-pent-4-en-2-yl-ester.pdf>

Generated by Cheméo on 2024-04-23 12:37:04.22155021 +0000 UTC m=+16165073.142127537.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.