

Adipic acid, di(pent-4-en-2-yl) ester

Inchi:	InChI=1S/C16H26O4/c1-5-9-13(3)19-15(17)11-7-8-12-16(18)20-14(4)10-6-2/h5-6,13-14H
InchiKey:	DVDZMSV FHVJCEH-UHFFFAOYSA-N
Formula:	C16H26O4
SMILES:	<chem>C=CCC(C)OC(=O)CCCC(=O)OC(C)CC=C</chem>
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	-213.20	kJ/mol	Joback Method
hf	-622.87	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.562		Crippen Method
mvol	242.580	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1791.00		NIST Webbook
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tb	710.54	K	Joback Method
tc	894.58	K	Joback Method
tf	380.88	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.62	J/molxK	710.54	Joback Method
cpg	757.04	J/molxK	863.90	Joback Method
cpg	744.39	J/molxK	833.23	Joback Method
cpg	730.93	J/molxK	802.56	Joback Method
cpg	716.67	J/molxK	771.89	Joback Method
cpg	701.57	J/molxK	741.21	Joback Method
cpg	768.90	J/molxK	894.58	Joback Method
dvisc	0.0000884	Paxs	710.54	Joback Method

dvisc	0.0001187	Paxs	655.60	Joback Method
dvisc	0.0001682	Paxs	600.65	Joback Method
dvisc	0.0002557	Paxs	545.71	Joback Method
dvisc	0.0004269	Paxs	490.77	Joback Method
dvisc	0.0008112	Paxs	435.82	Joback Method
dvisc	0.0018549	Paxs	380.88	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=U354134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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