

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

Inchi:	InChI=1S/C16H28O4/c1-4-6-9-13-19-15(17)11-7-8-12-16(18)20-14(3)10-5-2/h5,14H,2,4,
InchiKey:	HMHVUQQWRHWDUMU-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	C=CCC(C)OC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-298.60	kJ/mol	Joback Method
hf	-743.02	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mvol	246.880	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1870.00		NIST Webbook
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tb	714.30	K	Joback Method
tc	894.16	K	Joback Method
tf	397.64	K	Joback Method
vc	0.955	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.52	J/molxK	714.30	Joback Method
cpg	725.77	J/molxK	744.28	Joback Method
cpg	741.19	J/molxK	774.25	Joback Method
cpg	755.79	J/molxK	804.23	Joback Method
cpg	769.59	J/molxK	834.21	Joback Method
cpg	782.59	J/molxK	864.18	Joback Method
cpg	794.81	J/molxK	894.16	Joback Method
dvisc	0.0015131	Paxs	397.64	Joback Method

dvisc	0.0007187	Paxs	450.42	Joback Method
dvisc	0.0003991	Paxs	503.19	Joback Method
dvisc	0.0002478	Paxs	555.97	Joback Method
dvisc	0.0001671	Paxs	608.75	Joback Method
dvisc	0.0001200	Paxs	661.52	Joback Method
dvisc	0.0000905	Paxs	714.30	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=U354120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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