

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

Inchi:	InChI=1S/C17H30O4/c1-4-6-7-10-14-20-16(18)12-8-9-13-17(19)21-15(3)11-5-2/h5,15H,2
InchiKey:	OUIYVRMGRZVNBY-UHFFFAOYSA-N
Formula:	C17H30O4
SMILES:	C=CCC(C)OC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-290.18	kJ/mol	Joback Method
hf	-763.66	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.178		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1965.00		NIST Webbook
tb	737.18	K	Joback Method
tc	917.39	K	Joback Method
tf	408.91	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.33	J/molxK	737.18	Joback Method
cpg	782.97	J/molxK	767.22	Joback Method
cpg	798.75	J/molxK	797.25	Joback Method
cpg	813.66	J/molxK	827.29	Joback Method
cpg	827.74	J/molxK	857.32	Joback Method
cpg	840.98	J/molxK	887.36	Joback Method
cpg	853.40	J/molxK	917.39	Joback Method
dvisc	0.0013750	Paxs	408.91	Joback Method
dvisc	0.0006455	Paxs	463.62	Joback Method

dvisc	0.0003555	Paxs	518.33	Joback Method
dvisc	0.0002194	Paxs	573.04	Joback Method
dvisc	0.0001473	Paxs	627.76	Joback Method
dvisc	0.0001054	Paxs	682.47	Joback Method
dvisc	0.0000793	Paxs	737.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354122&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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