

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-292.62	kJ/mol	Joback Method
hf	-768.94	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpola	1922.00		NIST Webbook
tb	736.74	K	Joback Method
tc	918.83	K	Joback Method
tf	393.91	K	Joback Method
vc	1.004	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.82	J/molxK	736.74	Joback Method
cpg	783.65	J/molxK	767.09	Joback Method
cpg	799.59	J/molxK	797.44	Joback Method
cpg	814.65	J/molxK	827.78	Joback Method
cpg	828.83	J/molxK	858.13	Joback Method
cpg	842.16	J/molxK	888.48	Joback Method
cpg	854.64	J/molxK	918.83	Joback Method
dvisc	0.0016896	Paxs	393.91	Joback Method
dvisc	0.0007187	Paxs	451.05	Joback Method

dvisc	0.0003705	Paxs	508.19	Joback Method
dvisc	0.0002183	Paxs	565.33	Joback Method
dvisc	0.0001418	Paxs	622.46	Joback Method
dvisc	0.0000990	Paxs	679.60	Joback Method
dvisc	0.0000731	Paxs	736.74	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=U354121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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