

Adipic acid, isohexyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C18H32O4/c1-4-5-6-9-14-21-17(19)12-7-8-13-18(20)22-15-10-11-16(2)3/h5-6,
InchiKey:	MNHKUIFPPUKJDE-AATRIKPKSA-N
Formula:	C18H32O4
SMILES:	CCC=CCCOC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-289.38	kJ/mol	Joback Method
hf	-792.51	kJ/mol	Joback Method
hfus	44.63	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.426		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinsol	2102.00		NIST Webbook
tb	767.54	K	Joback Method
tc	951.19	K	Joback Method
tf	416.86	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.70	J/molxK	767.54	Joback Method
cpg	842.72	J/molxK	798.15	Joback Method
cpg	858.83	J/molxK	828.76	Joback Method
cpg	874.04	J/molxK	859.37	Joback Method
cpg	888.37	J/molxK	889.97	Joback Method
cpg	901.84	J/molxK	920.58	Joback Method
cpg	914.48	J/molxK	951.19	Joback Method
dvisc	0.0011565	Paxs	416.86	Joback Method
dvisc	0.0005130	Paxs	475.31	Joback Method

dvisc	0.0002719	Paxs	533.75	Joback Method
dvisc	0.0001633	Paxs	592.20	Joback Method
dvisc	0.0001075	Paxs	650.65	Joback Method
dvisc	0.0000758	Paxs	709.09	Joback Method
dvisc	0.0000564	Paxs	767.54	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=U354010&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

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