

Adipic acid, di(trans-hex-3-enyl) ester

Inchi:	InChI=1S/C18H30O4/c1-3-5-7-11-15-21-17(19)13-9-10-14-18(20)22-16-12-8-6-4-2/h5-8H
InchiKey:	GFIBZMYJRJLBF-KQQUZDAGSA-N
Formula:	C18H30O4
SMILES:	CCC=CCCOC(=O)CCCCC(=O)OCCC=CCC
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-206.72	kJ/mol	Joback Method
hf	-670.01	kJ/mol	Joback Method
hfus	48.35	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.346		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpola	2135.00		NIST Webbook
tb	772.14	K	Joback Method
tc	958.03	K	Joback Method
tf	426.78	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.69	J/molxK	772.14	Joback Method
cpg	817.04	J/molxK	803.12	Joback Method
cpg	832.51	J/molxK	834.10	Joback Method
cpg	847.15	J/molxK	865.08	Joback Method
cpg	860.98	J/molxK	896.06	Joback Method
cpg	874.02	J/molxK	927.05	Joback Method
cpg	886.32	J/molxK	958.03	Joback Method
dvisc	0.0008949	Paxs	426.78	Joback Method
dvisc	0.0004226	Paxs	484.34	Joback Method

dvisc	0.0002341	Paxs	541.90	Joback Method
dvisc	0.0001452	Paxs	599.46	Joback Method
dvisc	0.0000979	Paxs	657.02	Joback Method
dvisc	0.0000704	Paxs	714.58	Joback Method
dvisc	0.0000531	Paxs	772.14	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=U354023&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
mccvol:	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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