

Adipic acid, heptyl pent-4-enyl ester

Inchi:	InChI=1S/C18H32O4/c1-3-5-7-8-12-16-22-18(20)14-10-9-13-17(19)21-15-11-6-4-2/h4H,2
InchiKey:	JMCMLYANLGPJJS-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	C=CCCCOC(=O)CCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-279.32	kJ/mol	Joback Method
hf	-779.02	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinsol	2138.00		NIST Webbook
tb	760.50	K	Joback Method
tc	940.16	K	Joback Method
tf	435.18	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.69	J/molxK	760.50	Joback Method
cpg	899.29	J/molxK	910.22	Joback Method
cpg	885.90	J/molxK	880.27	Joback Method
cpg	871.66	J/molxK	850.33	Joback Method
cpg	856.55	J/molxK	820.39	Joback Method
cpg	840.57	J/molxK	790.44	Joback Method
cpg	911.85	J/molxK	940.16	Joback Method
dvisc	0.0000751	Paxs	760.50	Joback Method
dvisc	0.0000984	Paxs	706.28	Joback Method

dvisc	0.0001348	Paxs	652.06	Joback Method
dvisc	0.0001956	Paxs	597.84	Joback Method
dvisc	0.0003058	Paxs	543.62	Joback Method
dvisc	0.0005276	Paxs	489.40	Joback Method
dvisc	0.0010429	Paxs	435.18	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=U353796&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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