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

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

Physical Properties

Property code	Value	Unit	Source
gf	-281.76	kJ/mol	Joback Method
hf	-784.30	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.568		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	760.06	K	Joback Method
tc	941.19	K	Joback Method
tf	420.18	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.18	J/mol×K	760.06	Joback Method
cpg	841.21	J/mol×K	790.25	Joback Method
cpg	857.32	J/mol×K	820.44	Joback Method
cpg	872.53	J/mol×K	850.63	Joback Method
cpg	886.86	J/mol×K	880.81	Joback Method
cpg	900.31	J/mol×K	911.00	Joback Method
cpg	912.90	J/mol×K	941.19	Joback Method
dvisc	0.0012431	Pa×s	420.18	Joback Method

dvisc	0.0005770	Pa×s	476.83	Joback Method
dvisc	0.0003153	Pa×s	533.47	Joback Method
dvisc	0.0001934	Pa×s	590.12	Joback Method
dvisc	0.0001293	Pa×s	646.77	Joback Method
dvisc	0.0000922	Pa×s	703.41	Joback Method
dvisc	0.0000692	Pa×s	760.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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