Adipic acid, ethyl pent-4-enyl ester

Inchi: InChI=1S/C13H22O4/c1-3-5-8-11-17-13(15)10-7-6-9-12(14)16-4-2/h3H,1,4-11H2,2H3
InchiKey: YXGWLPLHOXJMFK-UHFFFAOYSA-N
Formula: C13H22O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-321.42	kJ/mol	Joback Method
hf	-675.82	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	646.10	K	Joback Method
tc	824.98	K	Joback Method
tf	378.83	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.83	J/mol×K	646.10	Joback Method
cpg	560.42	J/mol×K	675.91	Joback Method
cpg	574.33	J/mol×K	705.73	Joback Method
cpg	587.56	J/mol×K	735.54	Joback Method
cpg	600.14	J/mol×K	765.35	Joback Method
cpg	612.06	J/mol×K	795.17	Joback Method
cpg	623.32	J/mol×K	824.98	Joback Method
dvisc	0.0015761	Pa×s	378.83	Joback Method

dvisc	0.0008541	Pa×s	423.38	Joback Method
dvisc	0.0005201	Pa×s	467.92	Joback Method
dvisc	0.0003453	Pa×s	512.46	Joback Method
dvisc	0.0002447	Pa×s	557.01	Joback Method
dvisc	0.0001825	Pa×s	601.55	Joback Method
dvisc	0.0001417	Pa×s	646.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353790&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

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