Adipic acid, isobutyl pent-4-enyl ester

Inchi: InChI=1S/C15H26O4/c1-4-5-8-11-18-14(16)9-6-7-10-15(17)19-12-13(2)3/h4,13H,1,5-12H
InchiKey: JCBQGTWLNVAALE-UHFFFAOYSA-N
Formula: C15H26O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-307.02	kJ/mol	Joback Method
hf	-722.38	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.255		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	691.42	K	Joback Method
tc	871.43	K	Joback Method
tf	386.37	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.86	J/mol×K	691.42	Joback Method
cpg	669.68	J/mol×K	721.42	Joback Method
cpg	684.71	J/mol×K	751.42	Joback Method
cpg	698.97	J/mol×K	781.43	Joback Method
cpg	712.46	J/mol×K	811.43	Joback Method
cpg	725.19	J/mol×K	841.43	Joback Method
cpg	737.18	J/mol×K	871.43	Joback Method
dvisc	0.0016556	Pa×s	386.37	Joback Method

dvisc	0.0007963	Pa×s	437.21	Joback Method
dvisc	0.0004461	Pa×s	488.05	Joback Method
dvisc	0.0002788	Pa×s	538.89	Joback Method
dvisc	0.0001889	Pa×s	589.74	Joback Method
dvisc	0.0001362	Pa×s	640.58	Joback Method
dvisc	0.0001030	Pa×s	691.42	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=U353792&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