Succinic acid, cis-hex-3-enyl ethyl ester

Inchi: InChI=1S/C12H20O4/c1-3-5-6-7-10-16-12(14)9-8-11(13)15-4-2/h5-6H,3-4,7-10H2,1-2H3
InchiKey: WKZZFRSJSZINKQ-WAYWQWQTSA-N
Formula: C12H20O4
SMILES: CCC=CCCOC(=O)CCC(=O)OCC
Mol. weight [g/mol]: 228.28

Physical Properties

Property code	Value	Unit	Source
gf	-337.46	kJ/mol	Joback Method
hf	-663.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	630.70	K	Joback Method
tc	814.25	K	Joback Method
tf	364.24	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.03	J/mol×K	630.70	Joback Method
cpg	509.10	J/mol×K	661.29	Joback Method
cpg	522.51	J/mol×K	691.88	Joback Method
cpg	535.27	J/mol×K	722.48	Joback Method
cpg	547.40	J/mol×K	753.07	Joback Method
cpg	558.89	J/mol×K	783.66	Joback Method
cpg	569.75	J/mol×K	814.25	Joback Method
dvisc	0.0015837	Pa×s	364.24	Joback Method

dvisc	0.0008330	Pa×s	408.65	Joback Method
dvisc	0.0004970	Pa×s	453.06	Joback Method
dvisc	0.0003252	Pa×s	497.47	Joback Method
dvisc	0.0002281	Pa×s	541.88	Joback Method
dvisc	0.0001688	Pa×s	586.29	Joback Method
dvisc	0.0001303	Pa×s	630.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353403&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