

Succinic acid, heptyl pent-4-enyl ester

Inchi:	InChI=1S/C16H28O4/c1-3-5-7-8-10-14-20-16(18)12-11-15(17)19-13-9-6-4-2/h4H,2-3,5-1
InchiKey:	VSOQUBSBNFKWRJ-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	C=CCCCOC(=O)CCC(=O)OCCCCCCC
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-296.16	kJ/mol	Joback Method
hf	-737.74	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	1937.00		NIST Webbook
tb	714.74	K	Joback Method
tc	892.58	K	Joback Method
tf	412.64	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.04	J/molxK	714.74	Joback Method
cpg	781.35	J/molxK	862.94	Joback Method
cpg	768.44	J/molxK	833.30	Joback Method
cpg	754.77	J/molxK	803.66	Joback Method
cpg	740.32	J/molxK	774.02	Joback Method
cpg	725.08	J/molxK	744.38	Joback Method
cpg	793.49	J/molxK	892.58	Joback Method
dvisc	0.0000979	Paxs	714.74	Joback Method
dvisc	0.0001275	Paxs	664.39	Joback Method

dvisc	0.0001734	Paxs	614.04	Joback Method
dvisc	0.0002490	Paxs	563.69	Joback Method
dvisc	0.0003839	Paxs	513.34	Joback Method
dvisc	0.0006503	Paxs	462.99	Joback Method
dvisc	0.0012530	Paxs	412.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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