

Succinic acid, phenyl 6-chlorohexyl ester

Inchi:	InChI=1S/C16H21ClO4/c17-12-6-1-2-7-13-20-15(18)10-11-16(19)21-14-8-4-3-5-9-14/h3-
InchiKey:	SHAHIVFCWMQQOK-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	O=C(CCC(=O)Oc1ccccc1)OCCCCCCI
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-283.52	kJ/mol	Joback Method
hf	-642.38	kJ/mol	Joback Method
hfus	41.01	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.715		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinsol	2435.00		NIST Webbook
tb	782.17	K	Joback Method
tc	986.96	K	Joback Method
tf	470.74	K	Joback Method
vc	0.920	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.21	J/molxK	782.17	Joback Method
cpg	690.31	J/molxK	816.30	Joback Method
cpg	703.41	J/molxK	850.43	Joback Method
cpg	715.53	J/molxK	884.57	Joback Method
cpg	726.70	J/molxK	918.70	Joback Method
cpg	736.93	J/molxK	952.83	Joback Method
cpg	746.25	J/molxK	986.96	Joback Method
dvisc	0.0008477	Paxs	470.74	Joback Method
dvisc	0.0004737	Paxs	522.64	Joback Method

dvisc	0.0002941	Paxs	574.55	Joback Method
dvisc	0.0001976	Paxs	626.45	Joback Method
dvisc	0.0001411	Paxs	678.36	Joback Method
dvisc	0.0001057	Paxs	730.26	Joback Method
dvisc	0.0000822	Paxs	782.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357991&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
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

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