

Succinic acid, phenyl 2-methoxyethyl ester

Inchi:	InChI=1S/C13H16O5/c1-16-9-10-17-12(14)7-8-13(15)18-11-5-3-2-4-6-11/h2-6H,7-10H2,
InchiKey:	WWVZHSKHYBQNJR-UHFFFAOYSA-N
Formula:	C13H16O5
SMILES:	COCCOC(=O)CCC(=O)Oc1ccccc1
Mol. weight [g/mol]:	252.26

Physical Properties

Property code	Value	Unit	Source
gf	-401.85	kJ/mol	Joback Method
hf	-696.94	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	67.53	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.562		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinsol	1923.00		NIST Webbook
tb	698.52	K	Joback Method
tc	904.53	K	Joback Method
tf	429.24	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.51	J/molxK	698.52	Joback Method
cpg	574.50	J/molxK	870.20	Joback Method
cpg	564.28	J/molxK	835.86	Joback Method
cpg	553.17	J/molxK	801.53	Joback Method
cpg	541.17	J/molxK	767.19	Joback Method
cpg	528.28	J/molxK	732.86	Joback Method
cpg	583.82	J/molxK	904.53	Joback Method
dvisc	0.0001043	Paxs	698.52	Joback Method
dvisc	0.0001323	Paxs	653.64	Joback Method

dvisc	0.0001740	Paxs	608.76	Joback Method
dvisc	0.0002390	Paxs	563.88	Joback Method
dvisc	0.0003467	Paxs	519.00	Joback Method
dvisc	0.0005397	Paxs	474.12	Joback Method
dvisc	0.0009217	Paxs	429.24	Joback Method

Sources

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=U357986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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