

Succinic acid, 8-chlorooctyl cyclopentyl ester

Inchi: InChI=1S/C17H29ClO4/c18-13-7-3-1-2-4-8-14-21-16(19)11-12-17(20)22-15-9-5-6-10-15/
InchiKey: SEISXWLDJDSZDK-UHFFFAOYSA-N
Formula: C17H29ClO4
SMILES: O=C(CCC(=O)OC1CCCC1)OCCCCCCCCCl
Mol. weight [g/mol]: 332.86

Physical Properties

Property code	Value	Unit	Source
gf	-350.96	kJ/mol	Joback Method
hf	-839.07	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	76.39	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.375		Crippen Method
mvol	266.650	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	793.65	K	Joback Method
tc	989.44	K	Joback Method
tf	466.49	K	Joback Method
vc	1.026	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.20	J/molxK	793.65	Joback Method
cpg	831.05	J/molxK	826.28	Joback Method
cpg	846.82	J/molxK	858.91	Joback Method
cpg	861.51	J/molxK	891.55	Joback Method
cpg	875.16	J/molxK	924.18	Joback Method
cpg	887.79	J/molxK	956.81	Joback Method
cpg	899.43	J/molxK	989.44	Joback Method
dvisc	0.0011602	Paxs	466.49	Joback Method

dvisc	0.0006289	Paxs	521.02	Joback Method
dvisc	0.0003828	Paxs	575.54	Joback Method
dvisc	0.0002539	Paxs	630.07	Joback Method
dvisc	0.0001798	Paxs	684.60	Joback Method
dvisc	0.0001340	Paxs	739.12	Joback Method
dvisc	0.0001040	Paxs	793.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391383&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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