

Succinic acid, 8-chlorooctyl diphenylmethyl ester

Inchi:	InChI=1S/C25H31ClO4/c26-19-11-3-1-2-4-12-20-29-23(27)17-18-24(28)30-25(21-13-7-5
InchiKey:	RYWNQMXBFIVKPS-UHFFFAOYSA-N
Formula:	C25H31ClO4
SMILES:	O=C(CCC(=O)OC(c1ccccc1)c1ccccc1)OCCCCCCCCCl
Mol. weight [g/mol]:	430.96

Physical Properties

Property code	Value	Unit	Source
gf	-97.77	kJ/mol	Joback Method
hf	-596.89	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	98.10	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.222		Crippen Method
mvol	342.710	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	3271.00		NIST Webbook
rinpol	3271.00		NIST Webbook
tb	1014.33	K	Joback Method
tc	1245.11	K	Joback Method
tf	583.59	K	Joback Method
vc	1.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.24	J/molxK	1014.33	Joback Method
cpg	1114.58	J/molxK	1052.79	Joback Method
cpg	1126.51	J/molxK	1091.26	Joback Method
cpg	1137.12	J/molxK	1129.72	Joback Method
cpg	1146.48	J/molxK	1168.18	Joback Method
cpg	1154.65	J/molxK	1206.64	Joback Method
cpg	1161.72	J/molxK	1245.11	Joback Method
dvisc	0.0002974	Paxs	583.59	Joback Method

dvisc	0.0001492	Paxs	655.38	Joback Method
dvisc	0.0000857	Paxs	727.17	Joback Method
dvisc	0.0000544	Paxs	798.96	Joback Method
dvisc	0.0000372	Paxs	870.75	Joback Method
dvisc	0.0000270	Paxs	942.54	Joback Method
dvisc	0.0000205	Paxs	1014.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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