Succinic acid, 8-chlorooctyl phenethyl ester

Inchi: InChI=1S/C20H29ClO4/c21-15-8-3-1-2-4-9-16-24-19(22)12-13-20(23)25-17-14-18-10-6-5

InchiKey: JOTGGCGKNQGYDU-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: O=C(CCC(=O)OCCc1ccccc1)OCCCCCCCCCl

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-249.84	kJ/mol	Joback Method
hf	-724.94	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	85.09	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.675		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2834.00		NIST Webbook
rinpol	2834.00		NIST Webbook
tb	873.69	K	Joback Method
tc	1078.15	K	Joback Method
tf	515.82	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.78	J/mol×K	873.69	Joback Method
cpg	969.93	J/mol×K	1044.08	Joback Method
cpg	959.26	J/mol×K	1010.00	Joback Method
cpg	947.54	J/mol×K	975.92	Joback Method
cpg	934.75	J/mol×K	941.84	Joback Method
cpg	920.84	J/mol×K	907.77	Joback Method
cpg	979.58	J/mol×K	1078.15	Joback Method
dvisc	0.0000465	Pa×s	873.69	Joback Method

dvisc	0.0000605	Pa×s	814.04	Joback Method
dvisc	0.0000821	Pa×s	754.40	Joback Method
dvisc	0.0001173	Pa×s	694.75	Joback Method
dvisc	0.0001791	Pa×s	635.11	Joback Method
dvisc	0.0002988	Pa×s	575.47	Joback Method
dvisc	0.0005609	Pa×s	515.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U389754&Units=SI

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