Succinic acid, 2,4,6-trichlorophenyl 2-naphthylmethyl ester

Inchi: InChI=1S/C21H15Cl3O4/c22-16-10-17(23)21(18(24)11-16)28-20(26)8-7-19(25)27-12-13-

InchiKey: HCBQACBFVMQBOE-UHFFFAOYSA-N

Formula: C21H15Cl3O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 437.70

Physical Properties

Property code	Value	Unit	Source
gf	-84.74	kJ/mol	Joback Method
hf	-395.34	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	102.65	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.229		Crippen Method
mcvol	291.370	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	3407.00		NIST Webbook
rinpol	3407.00		NIST Webbook
tb	1037.01	K	Joback Method
tc	1288.96	K	Joback Method
tf	696.13	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.25	J/mol×K	1037.01	Joback Method
cpg	845.23	J/mol×K	1246.97	Joback Method
cpg	840.24	J/mol×K	1204.98	Joback Method
cpg	834.42	J/mol×K	1162.99	Joback Method
cpg	827.70	J/mol×K	1120.99	Joback Method
cpg	820.00	J/mol×K	1079.00	Joback Method
cpg	849.46	J/mol×K	1288.96	Joback Method
dvisc	0.0000695	Pa×s	1037.01	Joback Method

dvisc	0.0000827	Pa×s	980.20	Joback Method
dvisc	0.0001005	Pa×s	923.38	Joback Method
dvisc	0.0001253	Pa×s	866.57	Joback Method
dvisc	0.0001610	Pa×s	809.76	Joback Method
dvisc	0.0002150	Pa×s	752.94	Joback Method
dvisc	0.0003009	Pa×s	696.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390010&Units=SI
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

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