Succinic acid, naphth-2-ylmethyl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C21H16Cl2O4/c22-17-10-18(23)12-19(11-17)27-21(25)8-7-20(24)26-13-14-5-6

InchiKey: OFLHLJRUNDAELJ-UHFFFAOYSA-N

Formula: C21H16Cl2O4

SMILES: O=C(CCC(=O)Oc1cc(Cl)cc(Cl)c1)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 403.25

Physical Properties

Property code	Value	Unit	Source
gf	-63.18	kJ/mol	Joback Method
hf	-368.13	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	97.60	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	5.576		Crippen Method
mcvol	279.130	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	994.60	K	Joback Method
tc	1242.36	K	Joback Method
tf	653.69	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.99	J/mol×K	994.60	Joback Method
cpg	836.11	J/mol×K	1201.06	Joback Method
cpg	829.94	J/mol×K	1159.77	Joback Method
cpg	822.92	J/mol×K	1118.48	Joback Method
cpg	814.98	J/mol×K	1077.19	Joback Method
cpg	806.03	J/mol×K	1035.89	Joback Method
cpg	841.50	J/mol×K	1242.36	Joback Method
dvisc	0.0000788	Pa×s	994.60	Joback Method

dvisc	0.0000945	Pa×s	937.78	Joback Method
dvisc	0.0001160	Pa×s	880.96	Joback Method
dvisc	0.0001465	Pa×s	824.14	Joback Method
dvisc	0.0001915	Pa×s	767.33	Joback Method
dvisc	0.0002613	Pa×s	710.51	Joback Method
dvisc	0.0003764	Pa×s	653.69	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=U390160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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