Succinic acid, hept-2-yl 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C21H24Cl2O4/c1-3-4-5-8-14(2)26-19(24)11-12-20(25)27-21-16-10-7-6-9-15(16

InchiKey: YJRJFMNZGGZUFP-UHFFFAOYSA-N

Formula: C21H24Cl2O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 411.32

Physical Properties

Property code	Value	Unit	Source
gf	-178.03	kJ/mol	Joback Method
hf	-609.94	kJ/mol	Joback Method
hfus	50.48	kJ/mol	Joback Method
hvap	94.94	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.344		Crippen Method
mcvol	302.890	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	2986.00		NIST Webbook
rinpol	2986.00		NIST Webbook
tb	967.48	K	Joback Method
tc	1194.15	K	Joback Method
tf	612.27	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.73	J/mol×K	967.48	Joback Method
cpg	918.08	J/mol×K	1005.26	Joback Method
cpg	929.32	J/mol×K	1043.04	Joback Method
cpg	939.52	J/mol×K	1080.82	Joback Method
cpg	948.71	J/mol×K	1118.60	Joback Method
cpg	956.96	J/mol×K	1156.37	Joback Method
cpg	964.32	J/mol×K	1194.15	Joback Method
dvisc	0.0004101	Pa×s	612.27	Joback Method

dvisc	0.0002667	Pa×s	671.47	Joback Method
dvisc	0.0001860	Pa×s	730.67	Joback Method
dvisc	0.0001369	Pa×s	789.88	Joback Method
dvisc	0.0001052	Pa×s	849.08	Joback Method
dvisc	0.0000836	Pa×s	908.28	Joback Method
dvisc	0.0000684	Pa×s	967.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389904&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