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

Inchi: InChI=1S/C21H22Cl2O4/c22-17-12-18(23)21(16-9-5-4-8-15(16)17)27-20(25)11-10-19(24

InchiKey: MPLPRNKMLLSLBL-UHFFFAOYSA-N

Formula: C21H22Cl2O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12)OCC1CCCCC1

Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-151.14	kJ/mol	Joback Method
hf	-550.34	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	95.75	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	5.956		Crippen Method
mcvol	292.030	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	3245.00		NIST Webbook
rinpol	3245.00		NIST Webbook
tb	987.47	K	Joback Method
tc	1230.82	K	Joback Method
tf	634.65	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.05	J/mol×K	987.47	Joback Method
cpg	909.23	J/mol×K	1028.03	Joback Method
cpg	920.02	J/mol×K	1068.59	Joback Method
cpg	929.49	J/mol×K	1109.15	Joback Method
cpg	937.71	J/mol×K	1149.70	Joback Method
cpg	944.75	J/mol×K	1190.26	Joback Method
cpg	950.67	J/mol×K	1230.82	Joback Method
dvisc	0.0004390	Pa×s	634.65	Joback Method

dvisc	0.0002912	Pa×s	693.45	Joback Method
dvisc	0.0002059	Pa×s	752.26	Joback Method
dvisc	0.0001531	Pa×s	811.06	Joback Method
dvisc	0.0001185	Pa×s	869.86	Joback Method
dvisc	0.0000948	Pa×s	928.67	Joback Method
dvisc	0.0000778	Pa×s	987.47	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=U389906&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

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