Sebacic acid, 2,4-dichloronaphth-1-yl pentyl ester

Inchi: InChI=1S/C25H32Cl2O4/c1-2-3-12-17-30-23(28)15-8-6-4-5-7-9-16-24(29)31-25-20-14-11

InchiKey: DREOFGBFUDNCRK-UHFFFAOYSA-N

Formula: C25H32Cl2O4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 467.43

Physical Properties

Property code	Value	Unit	Source
gf	-141.91	kJ/mol	Joback Method
hf	-687.22	kJ/mol	Joback Method
hfus	64.37	kJ/mol	Joback Method
hvap	104.23	kJ/mol	Joback Method
log10ws	-9.26		Crippen Method
logp	7.906		Crippen Method
mcvol	359.250	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	3596.00		NIST Webbook
rinpol	3596.00		NIST Webbook
tb	1059.44	K	Joback Method
tc	1297.06	K	Joback Method
tf	672.35	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.79	J/mol×K	1059.44	Joback Method
cpg	1158.13	J/mol×K	1099.04	Joback Method
cpg	1170.23	J/mol×K	1138.65	Joback Method
cpg	1181.17	J/mol×K	1178.25	Joback Method
cpg	1191.01	J/mol×K	1217.85	Joback Method
cpg	1199.84	J/mol×K	1257.45	Joback Method
cpg	1207.74	J/mol×K	1297.06	Joback Method
dvisc	0.0002573	Pa×s	672.35	Joback Method

dvisc	0.0001669	Pa×s	736.87	Joback Method
dvisc	0.0001160	Pa×s	801.38	Joback Method
dvisc	0.0000852	Pa×s	865.89	Joback Method
dvisc	0.0000653	Pa×s	930.41	Joback Method
dvisc	0.0000518	Pa×s	994.92	Joback Method
dvisc	0.0000422	Pa×s	1059.44	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=U354957&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