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

Inchi: InChI=1S/C24H30Cl2O4/c1-2-3-16-29-22(27)14-8-6-4-5-7-9-15-23(28)30-24-19-13-11-10

InchiKey: SBFOIQJJWGPMFT-UHFFFAOYSA-N

Formula: C24H30Cl2O4

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

Mol. weight [g/mol]: 453.40

Physical Properties

Property code	Value	Unit	Source
gf	-150.33	kJ/mol	Joback Method
hf	-666.58	kJ/mol	Joback Method
hfus	61.78	kJ/mol	Joback Method
hvap	102.00	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.516		Crippen Method
mcvol	345.160	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	3477.00		NIST Webbook
rinpol	3477.00		NIST Webbook
tb	1036.56	K	Joback Method
tc	1269.51	K	Joback Method
tf	661.08	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.11	J/mol×K	1036.56	Joback Method
cpg	1138.18	J/mol×K	1230.69	Joback Method
cpg	1129.48	J/mol×K	1191.86	Joback Method
cpg	1119.79	J/mol×K	1153.04	Joback Method
cpg	1109.04	J/mol×K	1114.21	Joback Method
cpg	1097.18	J/mol×K	1075.39	Joback Method
cpg	1145.97	J/mol×K	1269.51	Joback Method
dvisc	0.0000489	Pa×s	1036.56	Joback Method

dvisc	0.0000598	Pa×s	973.98	Joback Method
dvisc	0.0000750	Pa×s	911.40	Joback Method
dvisc	0.0000975	Pa×s	848.82	Joback Method
dvisc	0.0001320	Pa×s	786.24	Joback Method
dvisc	0.0001883	Pa×s	723.66	Joback Method
dvisc	0.0002873	Pa×s	661.08	Joback Method

Sources

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=U354956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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