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

Inchi: InChI=1S/C24H30Cl2O4/c1-17(2)16-29-22(27)13-7-5-3-4-6-8-14-23(28)30-24-19-12-10-9

InchiKey: SFPLINZZNPRKDT-UHFFFAOYSA-N

Formula: C24H30Cl2O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 453.40

Physical Properties

Property code	Value	Unit	Source
gf	-152.77	kJ/mol	Joback Method
hf	-671.86	kJ/mol	Joback Method
hfus	58.25	kJ/mol	Joback Method
hvap	101.61	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.372		Crippen Method
mcvol	345.160	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
tb	1036.12	K	Joback Method
tc	1269.45	K	Joback Method
tf	646.08	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.42	J/mol×K	1036.12	Joback Method
cpg	1097.42	J/mol×K	1075.01	Joback Method
cpg	1109.20	J/mol×K	1113.90	Joback Method
cpg	1119.85	J/mol×K	1152.78	Joback Method
cpg	1129.42	J/mol×K	1191.67	Joback Method
cpg	1137.98	J/mol×K	1230.56	Joback Method
cpg	1145.61	J/mol×K	1269.45	Joback Method
dvisc	0.0002985	Pa×s	646.08	Joback Method

dvisc	0.0001879	Pa×s	711.09	Joback Method
dvisc	0.0001279	Pa×s	776.09	Joback Method
dvisc	0.0000923	Pa×s	841.10	Joback Method
dvisc	0.0000699	Pa×s	906.11	Joback Method
dvisc	0.0000549	Pa×s	971.11	Joback Method
dvisc	0.0000444	Pa×s	1036.12	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=U354955&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