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

Inchi: InChI=1S/C22H26Cl2O4/c1-2-27-20(25)13-7-5-3-4-6-8-14-21(26)28-22-17-12-10-9-11-16

InchiKey: TVUMIAIWXWZKMG-UHFFFAOYSA-N

Formula: C22H26Cl2O4

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

Mol. weight [g/mol]: 425.35

Physical Properties

Property code	Value	Unit	Source
gf	-167.17	kJ/mol	Joback Method
hf	-625.30	kJ/mol	Joback Method
hfus	56.60	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.736		Crippen Method
mcvol	316.980	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	990.80	K	Joback Method
tc	1217.56	K	Joback Method
tf	638.54	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.32	J/mol×K	990.80	Joback Method
cpg	976.87	J/mol×K	1028.59	Joback Method
cpg	988.32	J/mol×K	1066.39	Joback Method
cpg	998.72	J/mol×K	1104.18	Joback Method
cpg	1008.12	J/mol×K	1141.97	Joback Method
cpg	1016.58	J/mol×K	1179.77	Joback Method
cpg	1024.16	J/mol×K	1217.56	Joback Method
dvisc	0.0003551	Pa×s	638.54	Joback Method

dvisc	0.0002377	Pa×s	697.25	Joback Method
dvisc	0.0001694	Pa×s	755.96	Joback Method
dvisc	0.0001267	Pa×s	814.67	Joback Method
dvisc	0.0000986	Pa×s	873.38	Joback Method
dvisc	0.0000792	Pa×s	932.09	Joback Method
dvisc	0.0000652	Pa×s	990.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354953&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

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