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

Inchi: InChI=1S/C23H28Cl2O4/c1-2-15-28-21(26)13-7-5-3-4-6-8-14-22(27)29-23-18-12-10-9-11

InchiKey: NAPONDAPYAKGIZ-UHFFFAOYSA-N

Formula: C23H28Cl2O4

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

Mol. weight [g/mol]: 439.37

Physical Properties

Property code	Value	Unit	Source
gf	-158.75	kJ/mol	Joback Method
hf	-645.94	kJ/mol	Joback Method
hfus	59.19	kJ/mol	Joback Method
hvap	99.78	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.126		Crippen Method
mcvol	331.070	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	3374.00		NIST Webbook
tb	1013.68	K	Joback Method
tc	1243.03	K	Joback Method
tf	649.81	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.94	J/mol×K	1013.68	Joback Method
cpg	1077.10	J/mol×K	1204.81	Joback Method
cpg	1068.51	J/mol×K	1166.58	Joback Method
cpg	1058.97	J/mol×K	1128.36	Joback Method
cpg	1048.40	J/mol×K	1090.13	Joback Method
cpg	1036.74	J/mol×K	1051.91	Joback Method
cpg	1084.78	J/mol×K	1243.03	Joback Method
dvisc	0.0000565	Pa×s	1013.68	Joback Method
dvisc	0.0000688	Pa×s	953.04	Joback Method

dvisc	0.0000861	Pa×s	892.39	Joback Method
dvisc	0.0001113	Pa×s	831.75	Joback Method
dvisc	0.0001497	Pa×s	771.10	Joback Method
dvisc	0.0002119	Pa×s	710.46	Joback Method
dvisc	0.0003199	Pa×s	649.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354954&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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