

Sebacic acid, 2,5-dichlorophenyl isoheptyl ester

Inchi:	InChI=1S/C22H32Cl2O4/c1-17(2)10-9-15-27-21(25)11-7-5-3-4-6-8-12-22(26)28-20-16-18
InchiKey:	POQNVCCRQXACBS-UHFFFAOYSA-N
Formula:	C22H32Cl2O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	431.39

Physical Properties

Property code	Value	Unit	Source
gf	-266.63	kJ/mol	Joback Method
hf	-810.18	kJ/mol	Joback Method
hfus	56.44	kJ/mol	Joback Method
hvap	94.86	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.999		Crippen Method
mvol	336.440	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	2991.00		NIST Webbook
tb	966.40	K	Joback Method
tc	1184.62	K	Joback Method
tf	578.32	K	Joback Method
vc	1.300	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.77	J/molxK	966.40	Joback Method
cpg	1062.87	J/molxK	1002.77	Joback Method
cpg	1075.63	J/molxK	1039.14	Joback Method
cpg	1087.09	J/molxK	1075.51	Joback Method
cpg	1097.28	J/molxK	1111.88	Joback Method
cpg	1106.23	J/molxK	1148.25	Joback Method
cpg	1113.98	J/molxK	1184.62	Joback Method
dvisc	0.0002993	Paxs	578.32	Joback Method
dvisc	0.0001648	Paxs	643.00	Joback Method

dvisc	0.0001012	Paxs	707.68	Joback Method
dvisc	0.0000674	Paxs	772.36	Joback Method
dvisc	0.0000479	Paxs	837.04	Joback Method
dvisc	0.0000357	Paxs	901.72	Joback Method
dvisc	0.0000277	Paxs	966.40	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=U355090&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

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