Sebacic acid, 2,4-dichlorophenethyl isobutyl ester

Inchi: InChI=1S/C22H32Cl2O4/c1-17(2)16-28-22(26)10-8-6-4-3-5-7-9-21(25)27-14-13-18-11-12

InchiKey: DYLLJKZMAHQZRV-UHFFFAOYSA-N

Formula: C22H32Cl2O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl

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	-6.99		Crippen Method
logp	6.399		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	966.40	K	Joback Method
tc	1184.62	K	Joback Method
tf	578.32	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.77	J/mol×K	966.40	Joback Method
cpg	1062.87	J/mol×K	1002.77	Joback Method
cpg	1075.63	J/mol×K	1039.14	Joback Method
cpg	1087.09	J/mol×K	1075.51	Joback Method
cpg	1097.28	J/mol×K	1111.88	Joback Method
cpg	1106.23	J/mol×K	1148.25	Joback Method
cpg	1113.98	J/mol×K	1184.62	Joback Method
dvisc	0.0002993	Pa×s	578.32	Joback Method

dvisc	0.0001648	Pa×s	643.00	Joback Method
dvisc	0.0001012	Pa×s	707.68	Joback Method
dvisc	0.0000674	Pa×s	772.36	Joback Method
dvisc	0.0000479	Pa×s	837.04	Joback Method
dvisc	0.0000357	Pa×s	901.72	Joback Method
dvisc	0.0000277	Pa×s	966.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416817&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