

Sebacic acid, 4-chloro-3-methylphenyl isohexyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-18(2)11-10-16-27-22(25)12-8-6-4-5-7-9-13-23(26)28-20-14-15
InchiKey:	VMHOTQJALBALPO-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCCCCCCCC(=O)OCCCC(C)C)ccc1Cl</chem>
Mol. weight [g/mol]:	410.98

Physical Properties

Property code	Value	Unit	Source
gf	-246.28	kJ/mol	Joback Method
hf	-815.08	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	92.70	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.654		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpola	3044.00		NIST Webbook
tb	951.85	K	Joback Method
tc	1166.48	K	Joback Method
tf	559.67	K	Joback Method
vc	1.306	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.61	J/molxK	951.85	Joback Method
cpg	1100.12	J/molxK	987.62	Joback Method
cpg	1114.25	J/molxK	1023.39	Joback Method
cpg	1127.04	J/molxK	1059.16	Joback Method
cpg	1138.53	J/molxK	1094.93	Joback Method
cpg	1148.74	J/molxK	1130.70	Joback Method
cpg	1157.71	J/molxK	1166.48	Joback Method
dvisc	0.0003328	Paxs	559.67	Joback Method
dvisc	0.0001779	Paxs	625.03	Joback Method

dvisc	0.0001070	Paxs	690.40	Joback Method
dvisc	0.0000703	Paxs	755.76	Joback Method
dvisc	0.0000494	Paxs	821.12	Joback Method
dvisc	0.0000366	Paxs	886.49	Joback Method
dvisc	0.0000282	Paxs	951.85	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=U354847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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