

Sebacic acid, 2-(2-chlorophenoxy)ethyl pentyl ester

Inchi:	InChI=1S/C23H35ClO5/c1-2-3-12-17-28-22(25)15-8-6-4-5-7-9-16-23(26)29-19-18-27-21
InchiKey:	XCSAISTZYZVDSA-UHFFFAOYSA-N
Formula:	C23H35ClO5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCCOc1cccc1Cl
Mol. weight [g/mol]:	426.97

Physical Properties

Property code	Value	Unit	Source
gf	-339.21	kJ/mol	Joback Method
hf	-930.55	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	94.84	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.116		Crippen Method
mvol	344.160	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2950.00		NIST Webbook
rinpol	2950.00		NIST Webbook
tb	969.73	K	Joback Method
tc	1187.27	K	Joback Method
tf	584.38	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1113.61	J/molxK	969.73	Joback Method
cpg	1128.52	J/molxK	1005.99	Joback Method
cpg	1141.93	J/molxK	1042.24	Joback Method
cpg	1153.87	J/molxK	1078.50	Joback Method
cpg	1164.36	J/molxK	1114.75	Joback Method
cpg	1173.42	J/molxK	1151.01	Joback Method
cpg	1181.08	J/molxK	1187.27	Joback Method
dvisc	0.0002395	Paxs	584.38	Joback Method

dvisc	0.0001326	Paxs	648.61	Joback Method
dvisc	0.0000817	Paxs	712.83	Joback Method
dvisc	0.0000545	Paxs	777.06	Joback Method
dvisc	0.0000387	Paxs	841.28	Joback Method
dvisc	0.0000288	Paxs	905.50	Joback Method
dvisc	0.0000223	Paxs	969.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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