

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

Inchi:	InChI=1S/C29H47ClO5/c1-2-3-4-5-6-7-10-13-18-23-34-28(31)21-14-11-8-9-12-15-22-29
InchiKey:	MDNOKWIULWAYBZ-UHFFFAOYSA-N
Formula:	C29H47ClO5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]:	511.13

Physical Properties

Property code	Value	Unit	Source
gf	-288.69	kJ/mol	Joback Method
hf	-1054.39	kJ/mol	Joback Method
hfus	75.48	kJ/mol	Joback Method
hvap	108.19	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.457		Crippen Method
mvol	428.700	ml/mol	McGowan Method
pc	751.43	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	1107.01	K	Joback Method
tc	1374.89	K	Joback Method
tf	652.00	K	Joback Method
vc	1.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1484.65	J/molxK	1107.01	Joback Method
cpg	1500.71	J/molxK	1151.66	Joback Method
cpg	1514.33	J/molxK	1196.30	Joback Method
cpg	1525.60	J/molxK	1240.95	Joback Method
cpg	1534.61	J/molxK	1285.60	Joback Method
cpg	1541.43	J/molxK	1330.24	Joback Method
cpg	1546.16	J/molxK	1374.89	Joback Method
dvisc	0.0001112	Paxs	652.00	Joback Method

dvisc	0.0000582	Paxs	727.83	Joback Method
dvisc	0.0000344	Paxs	803.67	Joback Method
dvisc	0.0000223	Paxs	879.50	Joback Method
dvisc	0.0000155	Paxs	955.34	Joback Method
dvisc	0.0000113	Paxs	1031.17	Joback Method
dvisc	0.0000086	Paxs	1107.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U416780&Units=SI

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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