

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

Inchi:	InChI=1S/C22H33ClO5/c1-2-3-16-27-21(24)14-8-6-4-5-7-9-15-22(25)28-18-17-26-20-13
InchiKey:	DKUUCRFWZTZCLP-UHFFFAOYSA-N
Formula:	C22H33ClO5
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]:	412.95

Physical Properties

Property code	Value	Unit	Source
gf	-347.63	kJ/mol	Joback Method
hf	-909.91	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.726		Crippen Method
mvol	330.070	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	946.85	K	Joback Method
tc	1160.06	K	Joback Method
tf	573.11	K	Joback Method
vc	1.274	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.04	J/molxK	946.85	Joback Method
cpg	1067.79	J/molxK	982.38	Joback Method
cpg	1081.12	J/molxK	1017.92	Joback Method
cpg	1093.07	J/molxK	1053.45	Joback Method
cpg	1103.65	J/molxK	1088.99	Joback Method
cpg	1112.89	J/molxK	1124.52	Joback Method
cpg	1120.79	J/molxK	1160.06	Joback Method
dvisc	0.0002696	Paxs	573.11	Joback Method

dvisc	0.0001509	Paxs	635.40	Joback Method
dvisc	0.0000937	Paxs	697.69	Joback Method
dvisc	0.0000629	Paxs	759.98	Joback Method
dvisc	0.0000448	Paxs	822.27	Joback Method
dvisc	0.0000335	Paxs	884.56	Joback Method
dvisc	0.0000260	Paxs	946.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416773&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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