

Sebacic acid, 3-chlorophenethyl isobutyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-18(2)17-27-22(25)13-8-6-4-3-5-7-12-21(24)26-15-14-19-10-9
InchiKey:	VPUYCONCMYCKIY-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CC(C)COC(=O)CCCCCCCC(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-245.07	kJ/mol	Joback Method
hf	-782.97	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	89.81	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.746		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	923.99	K	Joback Method
tc	1134.49	K	Joback Method
tf	535.88	K	Joback Method
vc	1.250	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.82	J/molxK	923.99	Joback Method
cpg	1040.24	J/molxK	959.07	Joback Method
cpg	1054.38	J/molxK	994.16	Joback Method
cpg	1067.27	J/molxK	1029.24	Joback Method
cpg	1078.94	J/molxK	1064.32	Joback Method
cpg	1089.43	J/molxK	1099.41	Joback Method
cpg	1098.78	J/molxK	1134.49	Joback Method
dvisc	0.0004300	Paxs	535.88	Joback Method

dvisc	0.0002211	Paxs	600.57	Joback Method
dvisc	0.0001294	Paxs	665.25	Joback Method
dvisc	0.0000832	Paxs	729.93	Joback Method
dvisc	0.0000575	Paxs	794.62	Joback Method
dvisc	0.0000421	Paxs	859.30	Joback Method
dvisc	0.0000321	Paxs	923.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416238&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

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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