Sebacic acid, butyl 3-chlorophenethyl ester

Inchi: InChI=1S/C22H33ClO4/c1-2-3-16-26-21(24)13-8-6-4-5-7-9-14-22(25)27-17-15-19-11-10-
InchiKey: FOTNTOJJZDBEKF-UHFFFAOYSA-N
Formula: C22H33ClO4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-242.63	kJ/mol	Joback Method
hf	-777.69	kJ/mol	Joback Method
hfus	56.16	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.890		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	924.43	K	Joback Method
tc	1134.12	K	Joback Method
tf	550.88	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.36	J/mol×K	924.43	Joback Method
cpg	1039.76	J/mol×K	959.38	Joback Method
cpg	1053.89	J/mol×K	994.33	Joback Method
cpg	1066.80	J/mol×K	1029.27	Joback Method
cpg	1078.52	J/mol×K	1064.22	Joback Method
cpg	1089.07	J/mol×K	1099.17	Joback Method
cpg	1098.50	J/mol×K	1134.12	Joback Method
dvisc	0.0003880	Pa×s	550.88	Joback Method

dvisc	0.0002123	Pa×s	613.14	Joback Method
dvisc	0.0001298	Pa×s	675.40	Joback Method
dvisc	0.0000862	Pa×s	737.65	Joback Method
dvisc	0.0000611	Pa×s	799.91	Joback Method
dvisc	0.0000454	Pa×s	862.17	Joback Method
dvisc	0.0000352	Pa×s	924.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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