Sebacic acid, 4-chloro-2-methylbenzyl isobutyl ester

Inchi: InChI=1S/C22H33ClO4/c1-17(2)15-26-21(24)10-8-6-4-5-7-9-11-22(25)27-16-19-12-13-20

InchiKey: TYMWATLVZORJBM-UHFFFAOYSA-N

Formula: C22H33ClO4

SMILES: Cc1cc(Cl)ccc1COC(=O)CCCCCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-254.70	kJ/mol	Joback Method
hf	-794.44	kJ/mol	Joback Method
hfus	52.25	kJ/mol	Joback Method
hvap	90.48	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.012		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	928.97	K	Joback Method
tc	1140.43	K	Joback Method
tf	548.40	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.02	J/mol×K	928.97	Joback Method
cpg	1039.35	J/mol×K	964.21	Joback Method
cpg	1053.36	J/mol×K	999.46	Joback Method
cpg	1066.11	J/mol×K	1034.70	Joback Method
cpg	1077.60	J/mol×K	1069.94	Joback Method
cpg	1087.88	J/mol×K	1105.19	Joback Method
cpg	1096.97	J/mol×K	1140.43	Joback Method
dvisc	0.0003736	Pa×s	548.40	Joback Method

dvisc	0.0002018	Pa×s	611.83	Joback Method
dvisc	0.0001224	Pa×s	675.26	Joback Method
dvisc	0.0000809	Pa×s	738.68	Joback Method
dvisc	0.0000570	Pa×s	802.11	Joback Method
dvisc	0.0000424	Pa×s	865.54	Joback Method
dvisc	0.0000328	Pa×s	928.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380586&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